– stacking motifs in dialkylbis5-[(E)-2-aryldiazen-1-yl]-2-hydroxybenzoatotin(IV) complexes

Linden, Anthony ; Basu Baul, Tushar S

Abstract: The diorganotin(IV) complexes of 5-[(E)-2-aryldiazen-1-yl]-2-hydroxybenzoic acid are of interest because of their structural diversity in the crystalline state and their interesting biological activity. The structures of dimethylbis2-hydroxy-5-[(E)-2-(4-methylphenyl)diazen-1-yl]benzoatotin(IV), [Sn(CH3)2(C14H11N2O3)2], and di-n-butylbis2-hydroxy-5-[(E)-2-(4-methylphenyl)diazen-1-yl]benzoatotin(IV) benzene hemisolvate, [Sn(C4H9)2(C14H11N2O3)2] · 0.5C6H6, exhibit the usual skew-trapezoidal bipyramidal coordination geometry observed for related complexes of this class. Each structure has two independent molecules of the SnIV complex in the asymmetric unit. In the dimethyltin structure, intermolecular O-H...O hydrogen bonds and a very weak Sn...O interaction link the independent molecules into dimers. The planar carboxylate ligands lend themselves to [pi]-[pi] stacking interactions and the diversity of supramolecular structural motifs formed by these interactions has been examined in detail for these two structures and four closely related analogues. While there are some recurring basic motifs amongst the observed stacking arrangements, such as dimers and step-like chains, variations through longitudinal slipping and inversion of the direction of the overlay add complexity. The [pi]-[pi] stacking motifs in the two title complexes are combinations of some of those observed in the other structures and are the most complex of the structures examined.

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π–π stacking motifs in dialkylbis{5-[(*E*)-2-aryldiazen-1-yl]-2-hydroxybenzoato}tin(IV) complexes

Anthony Linden[a]* and Tushar S. Basu Baul[b]

[a]Department of Chemistry, University of Zurich, Winterthurerstrasse 190, CH-8057 Zurich, Switzerland, and [b]Centre for Advanced Studies in Chemistry, North-Eastern Hill University, NEHU Permanent Campus, Umshing, Shillong 793 022, India. *Correspondence e-mail: anthony.linden@chem.uzh.ch

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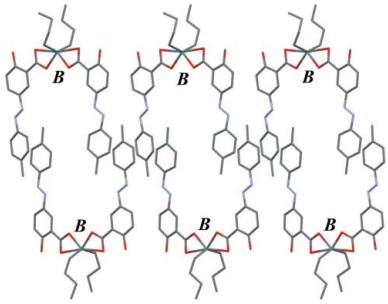
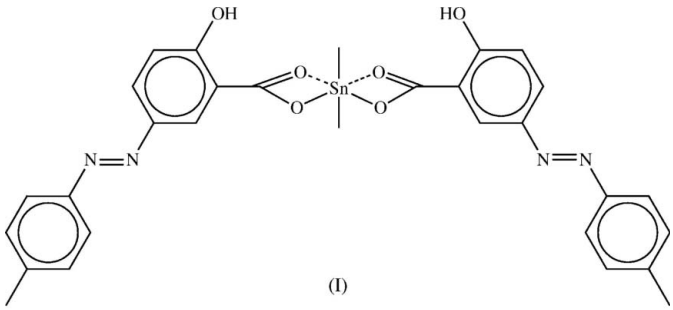
The diorganotin(IV) complexes of 5-[(*E*)-2-aryldiazen-1-yl]-2-hydroxybenzoic acid are of interest because of their structural diversity in the crystalline state and their interesting biological activity. The structures of dimethylbis{2-hydroxy-5-[(*E*)-2-(4-methylphenyl)diazen-1-yl]benzoato}tin(IV), $[Sn(CH_3)_2(C_{14}H_{11}N_2O_3)_2]$, and di-*n*-butylbis{2-hydroxy-5-[(*E*)-2-(4-methylphenyl)diazen-1-yl]benzoato}tin(IV) benzene hemisolvate, $[Sn(C_4H_9)_2(C_{14}H_{11}N_2O_3)_2]\cdot 0.5C_6H_6$, exhibit the usual skew-trapezoidal bipyramidal coordination geometry observed for related complexes of this class. Each structure has two independent molecules of the Sn^{IV} complex in the asymmetric unit. In the dimethyltin structure, intermolecular O—H···O hydrogen bonds and a very weak Sn···O interaction link the independent molecules into dimers. The planar carboxylate ligands lend themselves to π–π stacking interactions and the diversity of supramolecular structural motifs formed by these interactions has been examined in detail for these two structures and four closely related analogues. While there are some recurring basic motifs amongst the observed stacking arrangements, such as dimers and step-like chains, variations through longitudinal slipping and inversion of the direction of the overlay add complexity. The π–π stacking motifs in the two title complexes are combinations of some of those observed in the other structures and are the most complex of the structures examined.

1. Introduction

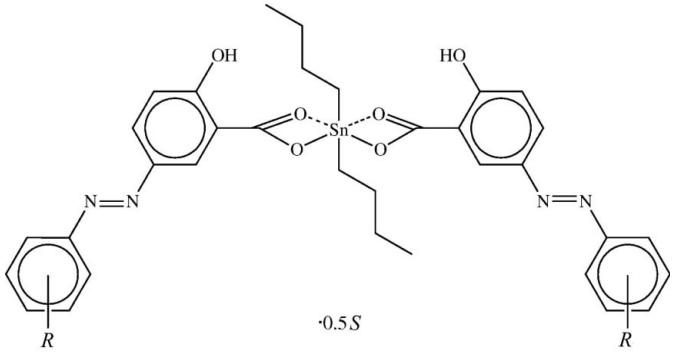
The diorganotin(IV) complexes of 5-[(*E*)-2-aryldiazen-1-yl]-2-hydroxybenzoic acid (*L*HH′) of the types (i) $R_2Sn(LH)_2$ [*R* = *n*-butyl (Bu) or *n*-octyl] (Basu Baul, Dhar & Tiekink, 2001; Basu Baul *et al.*, 2003, 2004, 2007; Linden *et al.*, 2007), (ii) $R_2Sn(LH)(L'H)$ [*R* = methyl (Me) or *n*-butyl; *L*′H has a different aryl group to *L*H] (Basu Baul *et al.*, 2005), and (iii) $\{[R_2Sn(LH)]_2O\}_2$ (Basu Baul *et al.*, 2006, 2007) are of interest because of their structural diversity in the crystalline state and their interesting biological activity (Basu Baul *et al.*, 2003, 2004, 2006). Earlier, a series of $Bu_2Sn(LH)_2$ complexes were examined where the carboxylate residue was varied by virtue of changes to the substitution of the terminal aryl group and the Bu_2Sn unit was held constant (Basu Baul *et al.*, 2004). The coordination geometries about the Sn^{IV} atoms in these complexes all show a similar skew-trapezoidal bipyramidal structural motif. We now report the crystal structures of dimethylbis{2-hydroxy-5-[(*E*)-2-(4-methylphenyl)diazen-1-yl]-benzoato}tin(IV), (I), and di-*n*-butylbis{2-hydroxy-5-[(*E*)-2-(4-methylphenyl)diazen-1-yl]benzoato}tin(IV) benzene hemisolvate, (II) (Scheme 1). These structures, in particular their π–π stacking motifs, are also compared with those of some closely related bis{5-[(*E*)-2-aryldiazen-1-yl]-2-hydroxybenzoato}dibutyltin(IV) complexes [aryl = phenyl, (IV); 3-methylphenyl,



(V); 4-bromophenyl, (VI)] and the ansolvate of (II), *i.e.* (III), that have been reported previously (Basu Baul *et al.*, 2004).



(I)



(II) R = 4-methyl, S = C_6H_6
(III) R = 4-methyl, S = nil
(IV) R = H, S = C_6H_6
(V) R = 3-methyl, S = C_6H_6
(VI) R = 4-Br, S = nil

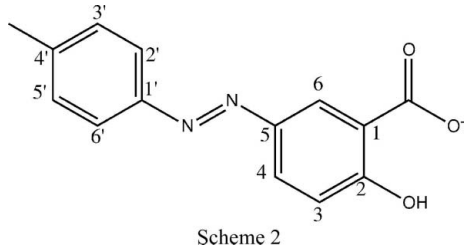
Scheme 1

2. Experimental

2.1. Synthesis and crystallization

Crystals of (I) and (II) were grown by slow evaporation of their solutions in benzene at room temperature. 2-Hydroxy-5-[(*E*)-2-(4-methylphenyl)diazen-1-yl]benzoic acid was prepared as described by Basu Baul, Dhar, Pyke *et al.* (2001). The preparation of compound (II) and its spectroscopic data are described by Basu Baul *et al.* (2004) (m.p. 447–449 K).

For the preparation of compound (I), Me_2SnCl_2 (0.19 g, 0.86 mmol) in anhydrous methanol (10 ml) was added dropwise with continuous stirring to a hot methanol solution (50 ml) containing sodium 2-hydroxy-5-[(*E*)-2-(4-methylphenyl)diazen-1-yl]benzoate (0.50 g, 1.79 mmol). The reaction mixture was then heated under reflux for 3 h and filtered while hot. The yellow-coloured filtrate was evaporated using a rotary evaporator and dried *in vacuo*. The residue was boiled with hexane to remove any unreacted Me_2SnCl_2. The residue was extracted into anhydrous benzene, filtered and concentrated to one third of its initial volume. The concentrated benzene solution was precipitated with hexane, which yielded the crude product. The precipitate was separated by filtration, washed with hexane (2 × 5 ml) and finally dried *in vacuo*. The dried product was then recrystallized from benzene, which furnished a yellow microcrystalline material in 72% yield (m.p. 493–495 K). The crystals of compound (I) used for single-crystal X-ray diffraction analysis had a melting point of 496–498 K. Analysis found: C 54.86, H 4.48, N 8.30%; calculated for $C_{30}H_{28}N_4O_6Sn$: C 54.66, H 4.28, N 8.50%. IR (KBr, cm^{-1}, p.p.m.): 1630 (*s*) $\nu(OCO)_{asym}$; 1590 (*s*), 1483 (*m*), 1416 (*s*) $\nu(OCO)_{sym}$; 1391 (*m*), 1296 (*m*), 1247 (*s*), 1203 (*m*), 1174 (*m*), 837 (*m*), 807 (*s*), 769 (*m*), 691 (*s*), 571 (*m*), 525 (*w*). ^{1}H NMR ($CDCl_3$, 300 MHz): δ_H 1.27 (*s*, 6H, Sn–CH_3), 2.44 (*s*, 6H, CH_3), 7.11 (*d*, 9.0 Hz, 2H, H3), 7.34 (*AA′* portion of *AA′XX′*, 4H, H2′ and H6′), 7.83 (*XX′*, portion of *AA′XX′*, 4H, H3′ and H5′), 8.12 (*dd*, 9.0 and 2.1 Hz, 2H, H4), 8.62 (*d*, 2.4 Hz, 2H, H6), 10.9 (*brs*, 2H, OH). ^{13}C NMR ($CDCl_3$, 75 MHz, p.p.m.): δ_C 5.47 (*s*, 6H, Sn–CH_3), 21.4 (CH_3), 112.5 (C1), 118.3 (C3), 122.7 (C2′ and C6′), 128.0 (C6), 129.3 (C4), 129.7 (C3 and C5′), 141.3 (C4′), 145.6 (C5), 150.6 (C1′), 163.6 (C2), 177.3 (CO_2); refer to Scheme 2 for the numbering protocol used for the NMR signal assignments. ^{119}Sn NMR ($CDCl_3$, p.p.m.): δ_{Sn} −84.8. ^{119}Sn Mössbauer parameters: δ 1.34; Δ 3.50; Γ_1 and Γ_2 1.0 mm s^{-1}.



Scheme 2

2.2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. The asymmetric unit of (II) contains two molecules of the Sn^{IV} complex, plus one molecule of benzene, while that of (I) also contains two molecules of the Sn^{IV} complex. For each structure, the atomic coordinates were tested carefully for a relationship to a higher symmetry space group using the program *PLATON* (Spek, 2009), but none could be found. In each independent molecule of the Sn^{IV} complex in the structure of (II), the outer three C atoms of one *n*-butyl group are disordered over two conformations. Refinement of the site-occupation factors for the two orientations yielded values of 0.718 (6) and 0.541 (5) for the major conformation of molecules *A* (containing atom Sn1) and *B* (containing atom Sn2), respectively. Similarity restraints were applied to the chemically equivalent bond lengths and angles of all C atoms in the *n*-butyl groups, including those of the ordered group in molecule *A*. In this way, the well defined geometry of the ordered *n*-butyl group helped to maintain reasonable geometry within the two conformations of the disordered ligands. The length of the first *n*-butyl C—C bond out from the Sn^{IV} atom was also restrained to 1.520 (5) Å. Neighbouring C atoms within and between each conformation of the disordered *n*-butyl groups were restrained to have similar atomic displacement parameters.

The hydroxy H atoms for (I) were located in a difference Fourier map and their positions were refined freely along with individual isotropic displacement parameters. The methyl H atoms in both models were constrained to an ideal geometry,

Table 1
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	$[Sn(CH_3)_2(C_{14}H_{11}N_2O_3)_2]$	$[Sn(C_4H_9)_2(C_{14}H_{11}N_2O_3)_2]\cdot 0.5C_6H_6$
M_r	659.25	1564.92
Crystal system, space group	Triclinic, $P\overline{1}$	Triclinic, $P\overline{1}$
Temperature (K)	160	160
a, b, c (Å)	10.1883 (1), 12.9209 (1), 23.0447 (2)	12.0462 (1), 13.6264 (2), 22.8143 (3)
α, β, γ (°)	102.3524 (4), 95.2584 (4), 104.1530 (5)	102.2665 (6), 100.3180 (6), 91.6029 (6)
V (Å^3)	2840.09 (4)	3591.71 (8)
Z	4	2
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.95	0.76
Crystal size (mm)	0.30 × 0.20 × 0.11	0.23 × 0.18 × 0.18
Data collection		
Diffractometer	Nonius KappaCCD	Nonius KappaCCD
Absorption correction	Multi-scan (Blessing, 1995)	Multi-scan (Blessing, 1995)
T_{min}, T_{max}	0.805, 0.912	0.802, 0.881
No. of measured, independent and observed $[I > 2\sigma(I)]$ reflections	69932, 16590, 10414	76914, 16442, 10227
R_{int}	0.070	0.083
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.704	0.650
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.041, 0.099, 1.01	0.046, 0.117, 1.03
No. of reflections	16590	16442
No. of parameters	763	971
No. of restraints	0	181
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.65, −1.07	1.58, −0.95

Computer programs: *COLLECT* (Nonius, 2000), *DENZO-SMN* (Otwinowski & Minor, 1997), *SCALEPACK* (Otwinowski & Minor, 1997), *SHELXS97* (Sheldrick, 2008), *ORTEPII* (Johnson, 1976), *SHELXL2014* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

with C—H = 0.98 Å and U_{iso}(H) = 1.5U_{eq}(C), but were allowed to rotate freely about the parent C—C bonds. The hydroxy groups of (II) were treated similarly, the O—H vector being aligned with peaks found in a difference Fourier map and with O—H = 0.84 Å. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.95 (aryl) or 0.99 Å (methylene) and U_{iso}(H) = 1.2U_{eq}(C).

3. Results and discussion

Compound (I) crystallizes with two molecules in the asymmetric unit (Fig. 1) while that in compound (II) has two molecules of the Sn^{IV} complex (Fig. 2) and one molecule of benzene (atoms C80–C85). There is no disorder in (I), but one of the *n*-butyl ligands in each independent molecule of (II) is disordered over two unequally occupied conformations (see *Experimental* details). The coordination geometry around the Sn^{IV} atom in each structure exhibits the typical skew-trapezoidal bipyramidal motif with no significant differences from the coordination geometries of the related analogues (III)–(VI) (Basu Baul *et al.*, 2004) (Scheme 1). The bidentate asymmetrically chelating carboxylate groups of two *L*H ligands form an equatorial plane around the Sn^{IV} atom. One carboxylate O atom of each ligand coordinates strongly to the Sn^{IV} atom, with Sn—O distances in the range 2.08–2.10 Å (Tables 2 and 3), while the second O atom coordinates more weakly, with Sn—O distances in the range 2.56–2.68 Å. The coordination is such that the strongly bound O atoms lie *cis* to one another, with a very acute O—Sn—O angle (*ca* 83°), while the weakly bound O atoms lie only *ca* 12° from being linearly disposed to one another, and consequently one side of the Sn^{IV} coordination sphere remains quite open. The coordinating C atoms of the alkyl groups lie in pseudo-axial positions, thereby completing six-coordination about the Sn^{IV} atom, but the C—Sn—C angle is distorted by 36–43° from a true *trans* position. This arrangement places the alkyl ligands somewhat over the open space left by the equatorial ligands to produce a skew-trapezoidal bipyramidal structure. The ranges of these geometric parameters demonstrate that the coordination geometries displayed by complexes (I) and (II) are thus extremely similar, except that the C—Sn—C angle appears to be very slightly smaller in (I) than in (II) (Tables 2 and 3).

The arrangement of the *n*-butyl ligands in (II) is unique compared with the other four dibutyltin analogues (Basu Baul *et al.*, 2004). In (II), both *n*-butyl ligands bend at the first CH_2 group such that the remainder of the ligand is directed away from and antiparallel to the longitudinal axis of the carboxylate ligands. In (III), the ansolvate analogue of (II), and the 4-bromophenyl derivative, (VI), only one *n*-butyl ligand adopts this conformation, while the other extends outward perpendicular to the plane of the carboxylate ligands. In the phenyl derivative, (IV), both *n*-butyl ligands extend out roughly perpendicular to the plane of the carboxylate ligands,

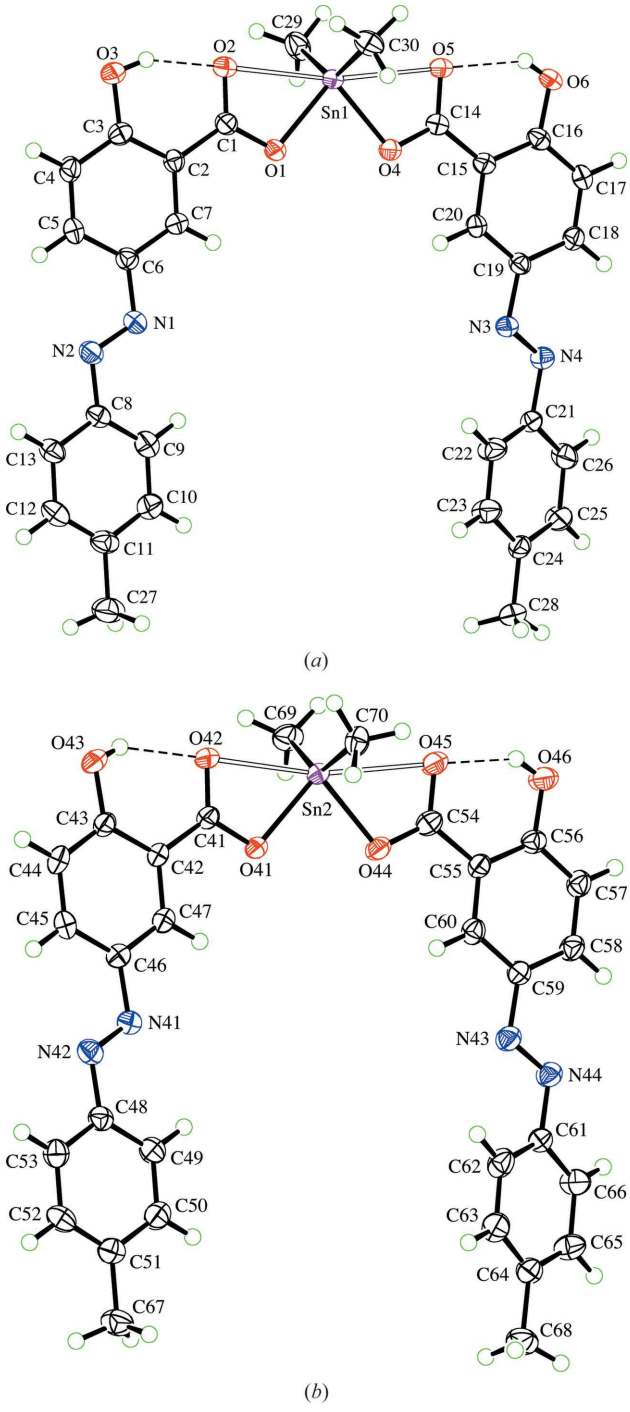


Figure 1
Views of the two symmetry-independent Sn^{IV} complex molecules of (I), *i.e.* (*a*) molecule *A* and (*b*) molecule *B*, showing the atom-labelling schemes. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary size. Open bonds represent the longer Sn—O bonds and thin dashed lines indicate intramolecular hydrogen bonds.

while in the 3-methylphenyl case, (V), one *n*-butyl ligand is perpendicular and one extends diagonally away from the plane of the carboxylate ligands.

The two symmetry-independent molecules in (I) have almost identical conformations, with an unweighted r.m.s. fit of the non-H atoms of 0.107 Å. In (II), the unweighted r.m.s. fit is

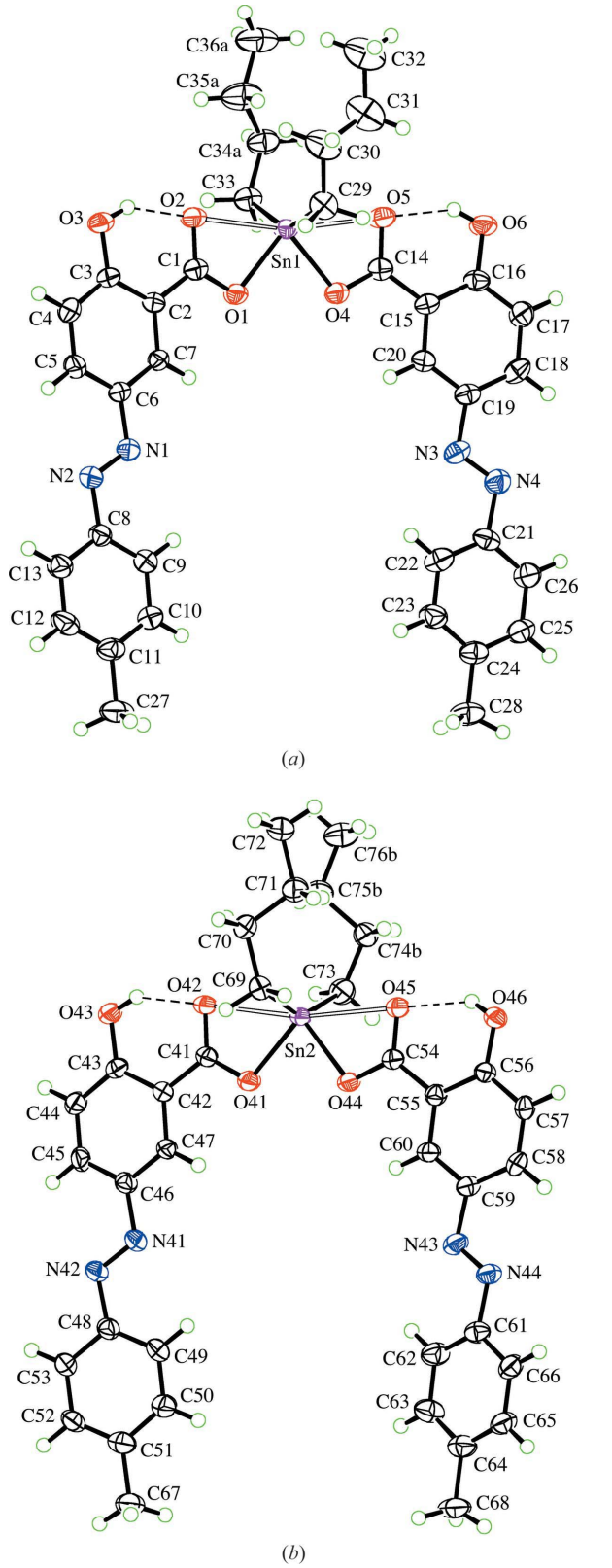


Figure 2
Views of the two symmetry-independent Sn^{IV} complex molecules of (II), *i.e.* (*a*) molecule *A* and (*b*) molecule *B*, showing the atom-labelling schemes. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary size. Open bonds represent the longer Sn—O bonds and thin dashed lines indicate intramolecular hydrogen bonds. The solvent benzene molecule has been omitted.

Table 2
Selected geometric parameters (Å, °) for (I).

Sn1—O1	2.0930 (17)	Sn2—O41	2.0966 (17)
Sn1—O2	2.6051 (18)	Sn2—O42	2.5613 (19)
Sn1—O4	2.0872 (17)	Sn2—O44	2.0855 (19)
Sn1—O5	2.6517 (18)	Sn2—O45	2.6798 (19)
Sn1—C29	2.089 (3)	Sn2—C69	2.093 (3)
Sn1—C30	2.090 (3)	Sn2—C70	2.095 (3)
O1—Sn1—O4	82.93 (7)	O41—Sn2—O44	83.06 (7)
O1—Sn1—O5	136.76 (6)	O41—Sn2—O45	136.67 (7)
O1—Sn1—C29	104.91 (10)	O41—Sn2—C69	107.65 (10)
O1—Sn1—C30	107.95 (10)	O41—Sn2—C70	105.62 (10)
O2—Sn1—O4	137.49 (7)	O42—Sn2—O44	138.31 (6)
O2—Sn1—O5	168.41 (6)	O42—Sn2—O45	168.07 (6)
O2—Sn1—C29	86.97 (10)	O42—Sn2—C69	90.91 (10)
O2—Sn1—C30	89.97 (10)	O42—Sn2—C70	89.12 (9)
O4—Sn1—C29	105.62 (11)	O44—Sn2—C69	103.72 (11)
O4—Sn1—C30	105.34 (10)	O44—Sn2—C70	103.02 (10)
O5—Sn1—C29	86.87 (10)	O45—Sn2—C69	84.44 (10)
O5—Sn1—C30	87.83 (10)	O45—Sn2—C70	87.28 (9)
C29—Sn1—C30	136.93 (12)	C69—Sn2—C70	139.25 (12)

Table 3
Selected geometric parameters (Å, °) for (II).

Sn1—O1	2.100 (2)	Sn2—O41	2.090 (2)
Sn1—O2	2.581 (2)	Sn2—O42	2.628 (2)
Sn1—O4	2.087 (2)	Sn2—O44	2.093 (2)
Sn1—O5	2.625 (3)	Sn2—O45	2.628 (2)
Sn1—C29	2.119 (3)	Sn2—C69	2.121 (3)
Sn1—C33	2.117 (3)	Sn2—C73	2.117 (3)
O1—Sn1—O4	83.18 (9)	O41—Sn2—O44	82.81 (9)
O1—Sn1—O5	137.43 (8)	O41—Sn2—O45	136.85 (8)
O1—Sn1—C29	100.36 (12)	O41—Sn2—C69	102.61 (11)
O1—Sn1—C33	106.03 (12)	O41—Sn2—C73	104.03 (11)
O2—Sn1—O4	138.10 (8)	O42—Sn2—O44	137.00 (8)
O2—Sn1—O5	167.32 (7)	O42—Sn2—O45	168.83 (7)
O2—Sn1—C29	86.01 (12)	O42—Sn2—C69	86.48 (11)
O2—Sn1—C33	89.64 (12)	O42—Sn2—C73	89.90 (11)
O4—Sn1—C29	101.81 (12)	O44—Sn2—C69	102.97 (12)
O4—Sn1—C33	104.98 (11)	O44—Sn2—C73	103.87 (12)
O5—Sn1—C29	88.16 (12)	O45—Sn2—C69	91.09 (11)
O5—Sn1—C33	88.50 (12)	O45—Sn2—C73	85.69 (11)
C29—Sn1—C33	144.16 (14)	C69—Sn2—C73	144.09 (13)

0.281 Å. The carboxylate ligands are nearly planar and coplanar with one another in each molecule in both complexes. The planes of the tolyl rings of each carboxylate ligand in each molecule in (I) are rotated slightly out of the plane of the remainder of the ligand, with this rotation being more significant for one arm of each ligand than in the other arm. The dihedral angles between the planes of the tolyl and 2-hydroxyphenyl rings of each arm of molecules *A* (containing atom Sn1) and *B* (containing atom Sn2) are 11.18 (14) and 22.57 (14)°, and 2.75 (14) and 19.28 (14)°, respectively, for the arms containing atoms O3, O6, O43 and O46. The corresponding dihedral angles in (II) are 2.91 (17), 8.07 (18), 3.42 (14) and 8.42 (17)°, respectively, demonstrating a much smaller deviation from coplanarity of the tolyl and 2-hydroxyphenyl rings. In the ansolvate of (II), these dihedral angles for the single unique molecule in the structure are 15.10 (12) and 9.43 (13)°, whereas in the phenyl and 3-methylphenyl derivatives, *i.e.* (IV) and (V), each carboxylate ligand is almost completely planar. In the 4-bromophenyl derivative, (VI), the corresponding dihedral angles are 19.22 (12) and 9.53 (11)° (Basu Baul *et al.*, 2004).

Within complexes (I) and (II) the diazenyl groups are arranged such that the C—N=N—C step points in opposite directions thereby increasing the distance between the terminal aryl groups relative to the distance between the 2-hydroxyphenyl rings and giving the appearance of an open tweezer. Such an arrangement is usually observed in the related structures, with exceptions being in the minor components of the disordered conformations in (IV) and (V) (Basu Baul *et al.*, 2004), where both C—N=N—C steps are in the same direction.

Structure (II) and its ansolvate (Basu Baul *et al.*, 2004) were both crystallized from benzene, and are thus pseudopolymorphs whose formation must depend subtly on the crystallization environment or rate, but such details were not recorded specifically. The former crystallized as isotropically shaped prisms, while the latter crystallized as very thin plates. The phenyl and 3-methylphenyl analogues crystallized as benzene hemisolvates, like (II), but with only one molecule of the Sn^{IV} complex in the asymmetric unit and the benzene molecules about centres of inversion. In the phenyl and 3-methylphenyl analogues, the benzene molecule lies between the arms of the carboxylate ligands and approximately perpendicular to and somewhat displaced from the plane occupied by these ligands; the distances from the mean plane through both 2-hydroxyphenyl rings of the ligands and the centroid of the benzene ring are approximately 3.41 and 1.65 Å, respectively. In (II), the benzene ring also lies between the arms of the carboxylate ligands of one of the independent Sn^{IV} complex molecules (molecule *A*), with the ring centroid

Table 4
Comparison of the unit-cell parameters of compounds (I)–(VI)[a].

	(I)	(II)	(III)	(IV)	(V)	(VI)
a (Å)	10.1883 (1)	12.0462 (1)	9.8270 (2)	11.6044 (1)	9.3399 (1)	9.6410 (1)
b (Å)	12.9209 (1)	13.6264 (2)	12.1642 (3)	11.5675 (1)	25.1934 (2)	12.1897 (2)
c (Å)	23.0447 (2)	22.8143 (3)	14.9382 (3)	25.9005 (3)	15.4687 (2)	15.1748 (2)
α (°)	102.3524 (4)	102.2665 (6)	93.357 (1)	90	90	94.1325 (7)
β (°)	95.2584 (4)	100.3180 (6)	100.016 (1)	97.3428 (4)	94.1425 (3)	98.7581 (7)
γ (°)	104.1530 (5)	91.6029 (6)	103.805 (1)	90	90	103.6085 (5)
V (Å^3)	2840.09 (4)	3591.71 (8)	1698.29 (7)	3448.21 (6)	3630.34 (7)	1702.24 (4)
Space group	$P\overline{1}$	$P\overline{1}$	$P\overline{1}$	$P2_1/c$	$P2_1/c$	$P\overline{1}$

Note: (*a*) details for compounds (III)–(VI) are taken from Basu Baul *et al.* (2004).

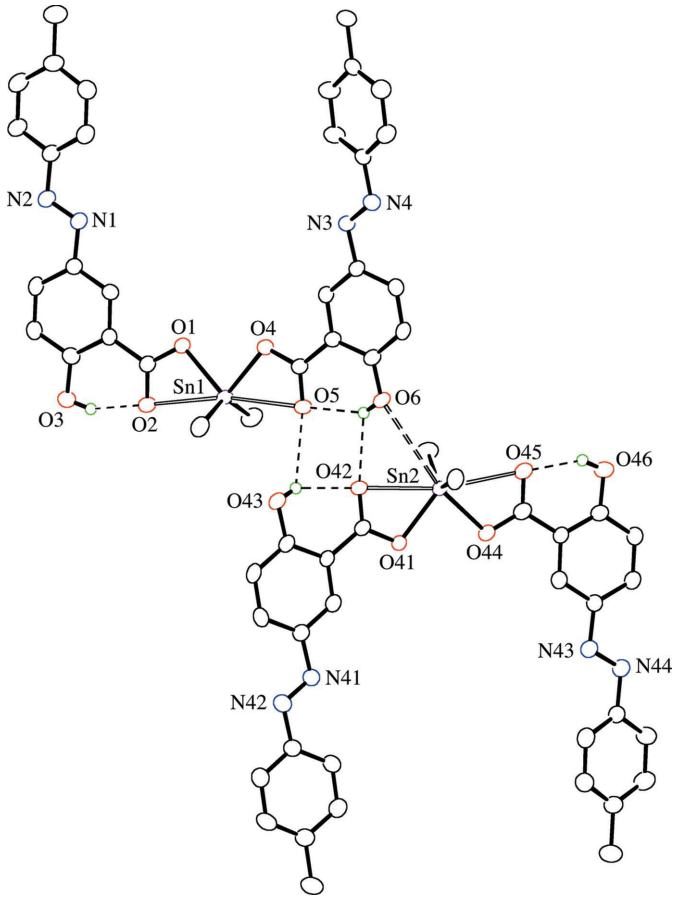


Figure 3
The head-to-head dimers in (I) formed by molecules *A* and *B*. Thin dashed lines represent hydrogen bonds, open bonds represent the longer Sn—O bonds of the Sn^{IV} coordination sphere and the open dashed bond indicates the long Sn2···O6 contact between the molecules. Displacement ellipsoids are drawn at the 50% probability level. Most H atoms have been omitted for clarity.

Table 5
Hydrogen-bond geometry (Å, °) for (I).

*Cg*5 and *Cg*7 are the centroids of the C42–C47 and C55–C60 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O2	0.80 (4)	1.89 (4)	2.611 (3)	150 (4)
O6—H6···O5	0.75 (3)	2.00 (3)	2.634 (3)	142 (4)
O6—H6···O42	0.75 (3)	2.35 (3)	2.887 (3)	130 (3)
O43—H43···O5	0.72 (3)	2.62 (3)	3.151 (3)	132 (3)
O43—H43···O42	0.72 (3)	2.01 (3)	2.642 (3)	146 (4)
O46—H46···O45	0.84 (3)	1.89 (3)	2.618 (3)	145 (3)
C29—H292···O43	0.98	2.37	3.314 (4)	162
C30—H303···O46^{i}	0.98	2.58	3.357 (4)	136
C68—H681···O44^{ii}	0.98	2.56	3.463 (4)	153
C69—H691···O2^{iii}	0.98	2.55	3.443 (4)	151
C12—H12···*Cg*7^{iv}	0.95	3.00	3.833 (3)	147
C68—H683···*Cg*5^{v}	0.98	2.86	3.625 (3)	136

Symmetry codes: (i) $x+1, y, z$; (ii) $-x-2, -y-1, -z$; (iii) $x-1, y, z$; (iv) $-x, -y+1, -z+1$; (v) $x-1, y-1, z$.

Table 6
Hydrogen-bond geometry (Å, °) for (II).

*Cg*4, *Cg*6, *Cg*7 and *Cg*9 are the centroids of the C21–C26, C48–C53, C55–C60 and C80–C86 (solvent benzene) rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O2	0.84	1.88	2.618 (3)	145
O6—H6···O5	0.84	1.89	2.631 (3)	146
O43—H43···O42	0.84	1.90	2.635 (3)	146
O46—H46···O45	0.84	1.91	2.627 (3)	142
C28—H281···O4^{vi}	0.98	2.56	3.385 (5)	142
C73—H733···O41^{vii}	0.99	2.58	3.540 (5)	162
C30—H301···*Cg*7	0.99	2.83	3.717 (5)	149
C34*A*—H341···*Cg*4^{viii}	0.99	2.64	3.586 (5)	160
C34*B*—H344···*Cg*4^{viii}	0.99	2.73	3.662 (13)	157
C70—H702···*Cg*6^{viii}	0.99	2.71	3.654 (4)	159
C74*A*—H741···*Cg*9^{vii}	0.99	2.69	3.643 (7)	161
C74*B*—H743···*Cg*9^{vii}	0.99	2.83	3.692 (7)	146

Symmetry codes: (vi) $-x+1, -y, -z$; (vii) $-x+1, -y+1, -z+1$; (viii) $x, y+1, z$.

about 2.17 Å from the mean plane through both 2-hydroxyphenyl rings of the ligands, but this time the benzene ring plane is essentially parallel to those of the carboxylate ligands. The other independent Sn^{IV} complex molecule also has its carboxylate ligand planes parallel to that of the benzene ring, but here the benzene ring is approximately over one 2-hydroxyphenyl ring, with a benzene centroid–hydroxyphenyl ring plane distance of 3.5404 (15) Å and a centroid–centroid distance of 3.680 (2) Å. In contrast, the planes of the carboxylate ligands of the two independent molecules in (I) are not parallel, but are inclined at an angle of approximately 42°. These aspects will be discussed below in conjunction with the description of the intermolecular interactions.

The 4-bromophenyl and ansolvated tolyl analogues have isomorphous triclinic unit cells and $Z' = 1$, while (I) and (II), both with two Sn^{IV} complex molecules in the asymmetric unit, are also triclinic, but with different unit-cell parameters, although these unit cells have quite similar metrics to one another (Table 4). As will be described below, the packing of the molecules in these two structures differs starkly. The monoclinic unit cells for the phenyl and 3-methylphenyl derivatives, both hemisolvates with $Z' = 1$, form another set with similar unit-cell volumes, although the unit-cell dimensions of the two are not very similar (Basu Baul *et al.*, 2004). There appears to be no clear correlation between the value of Z' and solvation in these six structures.

In (I) and (II), each 2-hydroxybenzoate hydroxy group forms an intramolecular hydrogen bond with the carboxylate carbonyl O atom of the same ligand (Tables 5 and 6). This interaction can be described by a graph-set motif of *S*(6) [see Bernstein *et al.* (1995) for a description of graph-set motifs].

The *n*-butyl ligands of each independent molecule in (II) fold back over the unoccupied side of the coordination polyhedron around the Sn^{IV} atom, and so any close approach of another molecule to the Sn^{IV} atom or the formation of intermolecular hydrogen bonds involving the hydroxy groups are precluded. In contrast, the less sterically demanding methyl ligands in (I) allow the close approach of another molecule and the formation of an intermolecular O—H···O hydrogen bond or even a very weak Sn···O interaction between the molecules, to give weakly associated head-to-head dimers (Fig. 3). Atom Sn2 (molecule *B*) is 3.529 (2) Å from hydroxy atom O6 (molecule *A*), which is just inside the sum of the van

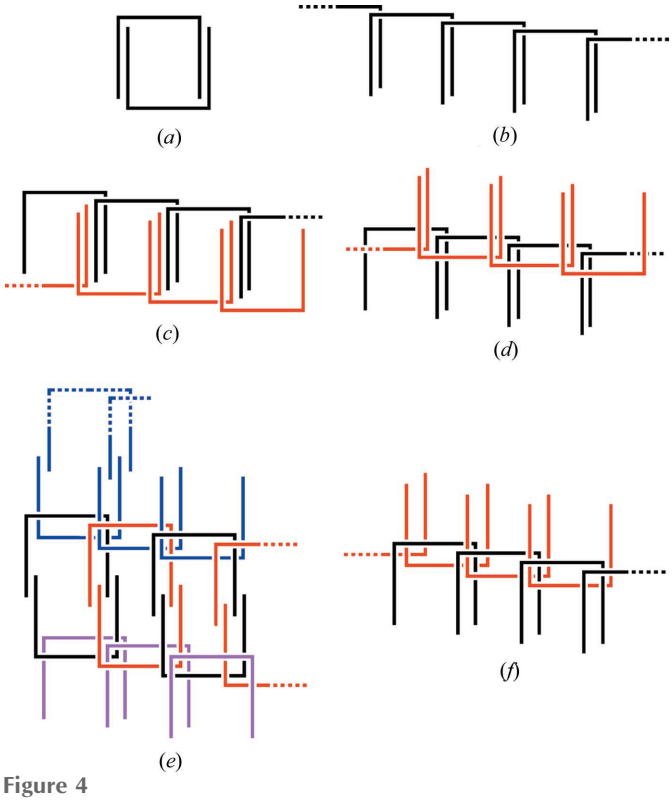


Figure 4
Cartoons of the π–π stacking motifs observed in the discussed structures, showing (*a*) the fully overlaid dimer motif in (V); (*b*) the fully overlaid stair-like chain motif in (III) and (IV), and as one of the two motifs in (I); (*c*) the fully overlaid inverted double-chain motif in (IV); (*d*) the longitudinally slipped inverted double-chain motif in (I); (*e*) the chain of partially overlaid dimer motifs within the complex arrangement in (II); (*f*) the double-chain motif in di-*n*-butylbis{2-hydroxy-5-[(*E*)-2-(2-methylphenyl)diazen-1-yl]benzoato}tin(IV).

der Waals radii of these atoms (*ca* 3.6 Å; Bondi, 1964). At the same time, this interaction is reinforced by an intermolecular hydrogen bond between the O6—H group in molecule *A* and carbonyl atom O42 of molecule *B* (Table 5). A similar O···Sn interaction involving atom Sn1 does not appear to exist; although the molecules are suitably aligned, the Sn1···O43 distance is 4.123 (2) Å and the O5···H43 distance is 2.61 (4) Å, which is marginally longer that that considered to be a significant hydrogen-bonding interaction. Similar interactions were observed in the structure of the phenyl analogue [Sn···O distance of 3.080 (2) Å], which resulted in the formation of chains of molecules, and in the structure of the 3-methylphenyl derivative [Sn···O distance of 3.439 (2) Å], where dimers are also present (Basu Baul *et al.*, 2004). If both intermolecular O—H···O interactions are considered, the *AB* dimers thus formed can be described by a graph-set motif of $R_2^2(12)$.

Weak C—H···O interactions do not play a major role in the supramolecular organization of (I) and (II). The O—H···O hydrogen-bonded dimer described above for (I) invokes a C—H···O interaction between the C29—H group of an Sn1-bound methyl group in molecule *A* and atom O43 in molecule *B*, although this might be a mere consequence of the above-described stronger interactions bringing these two molecules together (Table 5). The remaining C—H···O interactions listed in Table 5 are all quite long and involve methyl groups, so are likely to be so weak as to be almost negligible. There are no significant intermolecular C—H···O interactions in (II), with the shortest contacts involving methyl groups (Table 6).

The most striking supramolecular aggregation patterns in structures (I)–(VI) result from π–π stacking interactions. The carboxylate ligands with their two aryl rings and essentially planar extended conformation offer an excellent environment for molecules to assemble with their carboxylate ligands parallel to one another. Such interactions are found in all six structures. Several different motifs are formed by the assemblies and while some motifs recur across some of the structures, the complexity is greater for (I) and (II) than for the other four structures. Therefore, it is instructive to describe the π–π interaction motifs for structures (III)–(VI) first, as this will simplify the discussion of the interactions in (I) and (II). The supramolecular interactions of this kind in (III)–(VI) were not discussed in Basu Baul *et al.* (2004).

The simplest motif is observed for the 3-methylphenyl analogue, (V). Here the 'arms' formed by the carboxylate ligands of one molecule overlap in their entirety in an anti-parallel fashion with those of a single adjacent molecule to give a dimer. The π–π interactions occur between the 2-hydroxyphenyl ring of one ligand and the 3-methylphenyl ring of the adjacent ligand of the other molecule, and *vice versa* (Table 7). A cartoon representation of this motif is shown in Fig. 4(*a*). The structure is a benzene hemisolvate and the benzene molecule is encapsulated neatly within the internal cavity formed by the four carboxylate arms of the dimer. The next dimers each side of the primary dimer are offset, so that one of the carboxylate ligand arms lies over the cavity in the primary dimer, thus completing the encapsulation of the benzene molecule. The centrosymmetric benzene ring forms two significant symmetry-related C—H···π donor interactions with the 3-methylphenyl ring of these two capping ligands from adjacent dimers, but does not act as an acceptor of such interactions (C39—H39···*Cg*2^{ix}, with H···*Cg* = 2.77 Å and C—H···*Cg* = 145°; see Table 7 for the definition of all *Cg* and symmetry codes in this discussion).

For the 4-bromophenyl derivative, (VI), the arm of one carboxylate ligand overlaps in its entirety in a parallel fashion with the other carboxylate ligand in an adjacent molecule related to the first by translation along the [100] direction. The other carboxylate ligand in the primary molecule overlays similarly with another adjacent molecule on the other side. These interactions link the molecules into extended chains in which the carboxylate ligand arms always point in the same direction (Fig. 4*b*). The chains run parallel to [100] and the planes of the carboxylate ligands are tilted with respect to the axis of propagation to give a stair-like appearance. Significant π–π interactions are evident between adjacent 2-hydroxyphenyl rings, but adjacent 4-bromophenyl rings have much larger centroid–centroid distances and ring offsets, which suggests their interactions are almost negligible (Table 7). This could be related to the twist of the 4-bromophenyl ring plane from that of the remainder the ligand being larger for one

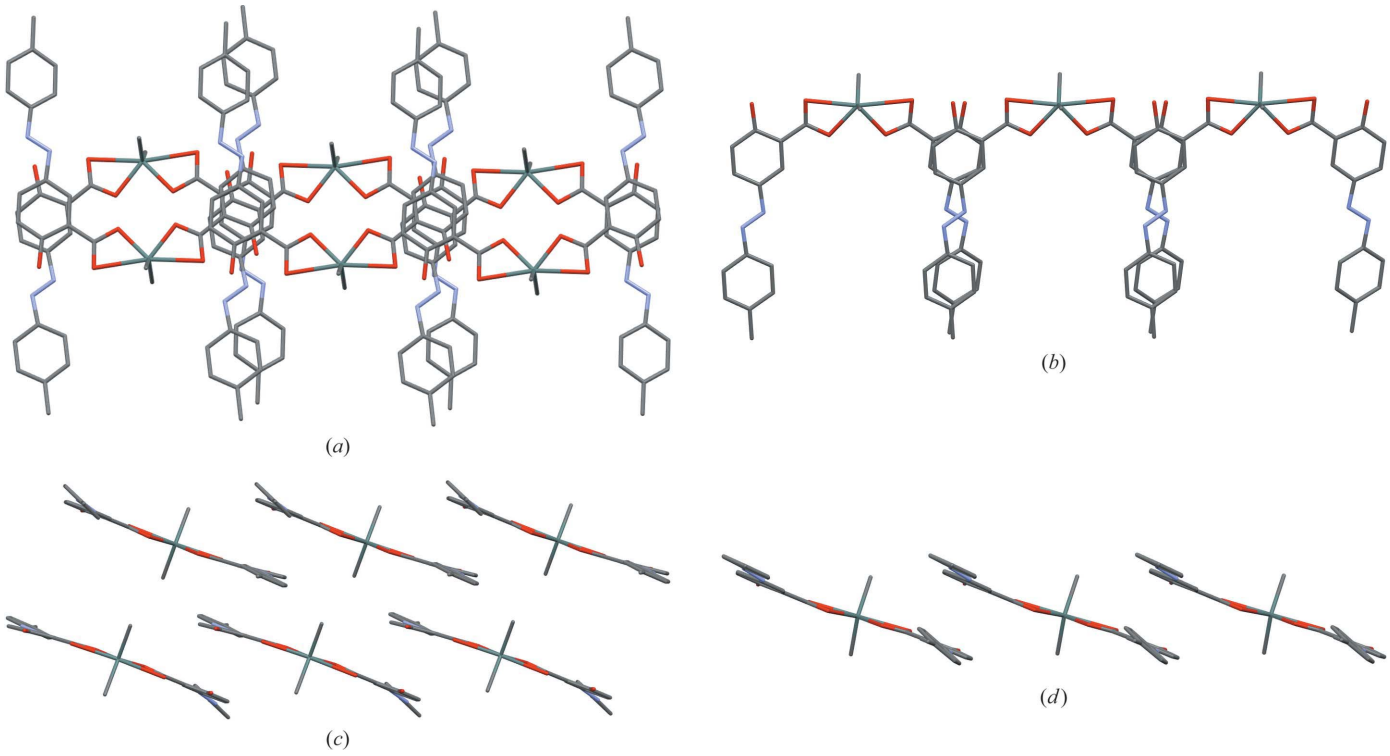


Figure 5
The π–π stacking of the molecules in (I), showing (*a*) the double chains resulting in short stacks of four overlapping carboxylate ligands formed by the *A* molecules, looking down the stacking direction; (*b*) a similar view showing the single chains of *B* molecules; (*c*)/(*d*) side views of (*a*) and (*b*), respectively. H atoms have been omitted for clarity and the [001] direction is horizontally across the diagram in all views.

ligand than for the other, as described above. One tolyl ring is capped on its other side by a C—H$\cdots\pi$ interaction involving an *n*-butyl ligand of a neighbouring chain (C32—H321$\cdots$*Cg*4^{vii}, with H$\cdots$*Cg* = 2.74 Å and C—H$\cdots$*Cg* = 154°).

The structure of (III), the ansolvate analogue of (II), shows an identical π–π interaction motif to (VI) (Fig. 4*b*), including the longer centroid–centroid and ring-offset distances between the similarly twisted tolyl rings (Table 7). These chains also run parallel to the [100] direction. Only a single pair of π–π interacting 2-hydroxyphenyl rings exists at any one location; a C—H$\cdots\pi$ interaction from *n*-butyl ligands of two different neighbouring chains caps one side of the carboxylate ligand in each pair involving *Cg*1 and *Cg*2 [C36—H361$\cdots$*Cg*1(x + 1, y + 1, z), with H$\cdots$*Cg* = 2.80 Å and C—H$\cdots$*Cg* = 149°, and C28—H282$\cdots$*Cg*2(−x + 1, −y, −z + 1), with H$\cdots$*Cg* = 2.74 Å and C—H$\cdots$*Cg* = 152°].

The phenyl analogue, (IV), has a more complex π–π interaction motif overall (Fig. 4*c*), but this can be constructed by starting with the same chain motif described for (III) and (VI). These chains run parallel to the [010] direction. In this case, the terminal phenyl rings are almost coplanar with the rest of their ligand, so their centroid-centroid and ring offset distances are more indicative of stronger π–π interactions. The difference to (II) and (VI) is that a second such chain, related to the first chain by a centre of inversion, lies on top of the first chain and interacts with it *via* very weak and offset π–π interactions between the opposing phenyl and 2-hydroxymethyl rings to give overall a double-thickness chain (Fig. 4*c*). The carboxylate ligands are somewhat longitudinally slipped by sliding of the 2-hydroxyphenyl rings slightly towards one another. This arrangement leads to short stacks of four π–π bonded carboxylate ligands, the first two being parallel to one another and antiparallel to the other two. Within each stack, the inner two carboxylate ligands are symmetry-related versions of the same unique ligand and their phenyl and 2-hydroxyphenyl rings thus have π–π interactions on both sides, whereas the corresponding rings of the outer carboxylate ligands involve the other symmetry-unique ligand and have π–π interactions only on one side. These stacks are capped on each end by the *n*-butyl ligands of molecules from adjacent chains. The benzene solvent molecule in this structure is encapsulated in cavities that exist within the double chain surrounded by two edge-on carboxylate ligands and two *n*-butyl ligands from four Sn^{IV} complex molecules, two from each chain.

In (I), with its two symmetry-independent molecules, two of the above-described chain motifs are found. The *A* molecules (containing atom Sn1) form a similar overlaid double-chain motif to that found for (IV) (Figs. 4*d* and 5*a*), while the *B* molecules (containing atom Sn2) adopt the single-chain motif found in (III) and (VI) (Figs. 4*b* and 5*b*). The main difference between the double-chain motif of (IV) and that for the *A* molecules of (I) is that the longitudinal slippage of the carboxylate ligand arms of the two single chains, which are related by a centre of inversion, is now much more severe, with the 2-hydroxypenyl rings now slipped even slightly beyond

Table 7
Geometry of the π–π interactions in compounds (I)–(VI) (Å, °).

Cg are the centroids of the 2-hydroxyphenyl and terminal aryl rings defined by the following atoms: *Cg*1 C2–C7; *Cg*2 C8–C13; *Cg*3 C15–C20; *Cg*4 C21–C26; *Cg*5 C42–C47; *Cg*6 C48–C53; *Cg*7 C55–C60; *Cg*8 C61–C66; *Cg*9 C80–C86 (solvent benzene). In structures with disordered carboxylate ligands, only the major conformation is considered. α is the dihedral angle between planes *I* and *J*, β is the angle between the *CgI*···*CgJ* vector and the normal to the plane *I*, γ is the angle between the *CgI*···*CgJ* vector and the normal to plane *J*, *CgI*···Plane*J* is the perpendicular distance of *CgI* from the plane of ring *J*, *CgJ*···Perp*I* is the perpendicular distance of *CgJ* from the plane of ring *I*, and the slippage is the distance between *CgI* and the perpendicular projection of *CgJ* on the plane of ring *I* (calculated with *PLATON*; Spek, 2009).

Interaction	*CgI*···*CgJ*	*CgI*···Plane*J*	*CgJ*···Plane*I*	α	β	γ	Slippage
Compound (I)							
*Cg*1···*Cg*1^{vii}	3.8578 (16)	3.5175 (11)	3.5174 (11)	0	24.3	24.3	1.59
*Cg*1···*Cg*3^{ix}	3.6778 (16)	3.4955 (11)	3.4628 (11)	7.28 (13)	19.7	18.1	1.24
*Cg*5···*Cg*7^{ix}	3.6492 (16)	3.4107 (11)	3.4990 (11)	4.65 (13)	16.5	20.8	1.04
Compound (II)							
*Cg*1···*Cg*1^{x}	4.082 (2)	3.6860 (14)	3.6861 (14)	0	25.4	25.4	1.75
*Cg*1···*Cg*3^{xi}	4.028 (2)	3.7388 (14)	3.7789 (15)	13.98 (17)	20.3	21.8	1.39
*Cg*2···*Cg*6^{vi}	3.780 (2)	3.5022 (15)	3.5833 (15)	6.24 (18)	18.5	22.1	1.20
*Cg*2···*Cg*8^{xii}	3.987 (2)	3.7113 (15)	3.8503 (15)	12.92 (18)	15.1	21.5	1.04
*Cg*3···*Cg*9	3.680 (2)	3.5404 (15)	3.505 (2)	4.5 (2)	17.8	15.8	1.12
*Cg*4···*Cg*8^{vi}	3.805 (2)	3.4786 (15)	3.5700 (15)	9.33 (18)	20.3	23.9	1.32
*Cg*5···*Cg*5^{xiii}	3.9809 (19)	3.6944 (14)	3.6945 (14)	0	21.9	21.9	1.48
*Cg*5···*Cg*7^{vii}	3.955 (2)	3.4673 (14)	3.5635 (14)	4.05 (16)	25.7	28.8	1.72
Compound (III)							
*Cg*1···*Cg*3^{iii}	3.6225 (14)	3.4408 (9)	3.4347 (10)	1.86 (11)	18.5	18.2	1.15
*Cg*2···*Cg*4^{iii}	4.1928 (15)	3.6557 (11)	3.4482 (11)	8.09 (13)	34.7	29.3	2.39
Compound (IV)							
*Cg*1···*Cg*3^{viii}	3.803 (9)	3.4525 (10)	3.440 (9)	0.5 (7)	25.2	24.8	1.62
*Cg*2···*Cg*4^{viii}	3.816 (7)	3.4796 (12)	3.488 (7)	3.6 (6)	23.9	24.2	1.55
*Cg*1···*Cg*2^{xiv}	4.1647 (16)	3.4726 (10)	3.5033 (12)	1.95 (13)	32.7	33.5	2.25
Compound (V)							
*Cg*1···*Cg*4^{xiii}	3.700 (6)	3.5000 (8)	3.481 (5)	4.1 (4)	19.8	19.0	1.25
*Cg*2···*Cg*3^{xiii}	3.799 (4)	3.5128 (8)	3.398 (4)	4.2 (3)	26.6	22.4	1.70
Compound (VI)							
*Cg*1···*Cg*3^{iii}	3.6310 (13)	3.4220 (10)	3.4344 (9)	3.21 (11)	18.9	19.5	1.18
*Cg*2···*Cg*4^{iii}	4.2534 (14)	3.6431 (11)	3.3332 (10)	7.43 (12)	38.4	31.1	2.64

Symmetry codes: (iii) $x-1, y, z$; (vi) $-x+1, -y, -z$; (vii) $-x+1, -y+1, -z+1$; (viii) $x, y+1, z$; (ix) $x+1, y, z$; (x) $-x, -y+1, -z$; (xi) $-x+1, -y+1, -z$; (xii) $-x, -y, -z$; (xiii) $-x+2, -y+1, -z+1$; (xiv) $-x+1, -y+2, -z+1$.

one another (Figs. 4*d* and 5*a*). Thus, only the 2-hydroxyphenyl rings from the two contributing chains overlay and the carboxylate ligands from the two constituent chains lie anti-parallel, with their arms extending out in opposite directions, thereby precluding π–π interactions between terminal tolyl rings. The short stacks of four π–π bonded 2-hydroxyphenyl rings are capped by C—H···π interactions (Table 5). Both types of chains run parallel to the [100] direction, but the tilts of the molecules with respect to the direction of propagation differ and thereby preclude additional π–π interactions between the *A* and *B* chains. Although the single-stranded *B* chains are one molecule thick, pairs of chains of *B* molecules run parallel to and lie between the chains of *A* molecules, but unlike the double thickness of the *A* chains, there are no significant interchain interactions between the adjacent chains of *B* molecules, because the methyl ligands protruding approximately perpendicular to the planes of the carboxylate ligands get in the way and cause the ligand arms of two chains that would otherwise form the double chain to be offset. This is something that does not appear to occur within the double chains of *A* molecules (Fig. 6*a*). The double chains of *A* molecules and pairs of chains of *B* molecules are stacked in an alternating sequence along the [01$\bar{1}$] direction. The intermolecular O—H···O hydrogen bonds between molecules *A* and *B*, described earlier, serve to crosslink adjacent *A* and *B* chains perpendicular to [01$\bar{1}$], thereby forming *A*+*B* ribbons along [100] with the hydrophilic ends of the carboxylate ligands facing towards the centre of the ribbon (Fig. 6*b*).

In (II), the planes containing the carboxylate ligands in the *A* (containing Sn1) and *B* molecules (with Sn2), as well as those of the benzene solvent molecules, all lie parallel in the structure, which permits an extensive and complex series of π–π interactions, albeit mostly quite weak, to build the supramolecular structure. Nevertheless, it is still possible to discern some of the above-described motifs. Firstly, the tolyl rings of molecule *A* (centres of gravity *Cg*2 and *Cg*4, as defined in Table 7) interact with the tolyl rings of molecule *B* (centres of gravity *Cg*6 and *Cg*8, respectively) at $(-x+1, -y, -z)$ to form a dimeric tail-to-tail pair (Fig. 4*e*, black or red motifs), in the cavity of which the solvent benzene molecule is located (Fig. 7*a*). This motif is similar to that described above for (V) (Fig. 4*a*), but with the overlap moved longitudinally along the carboxylate ligand arms so that only the tolyl rings overlap. Then the other sides of the tolyl rings on opposite

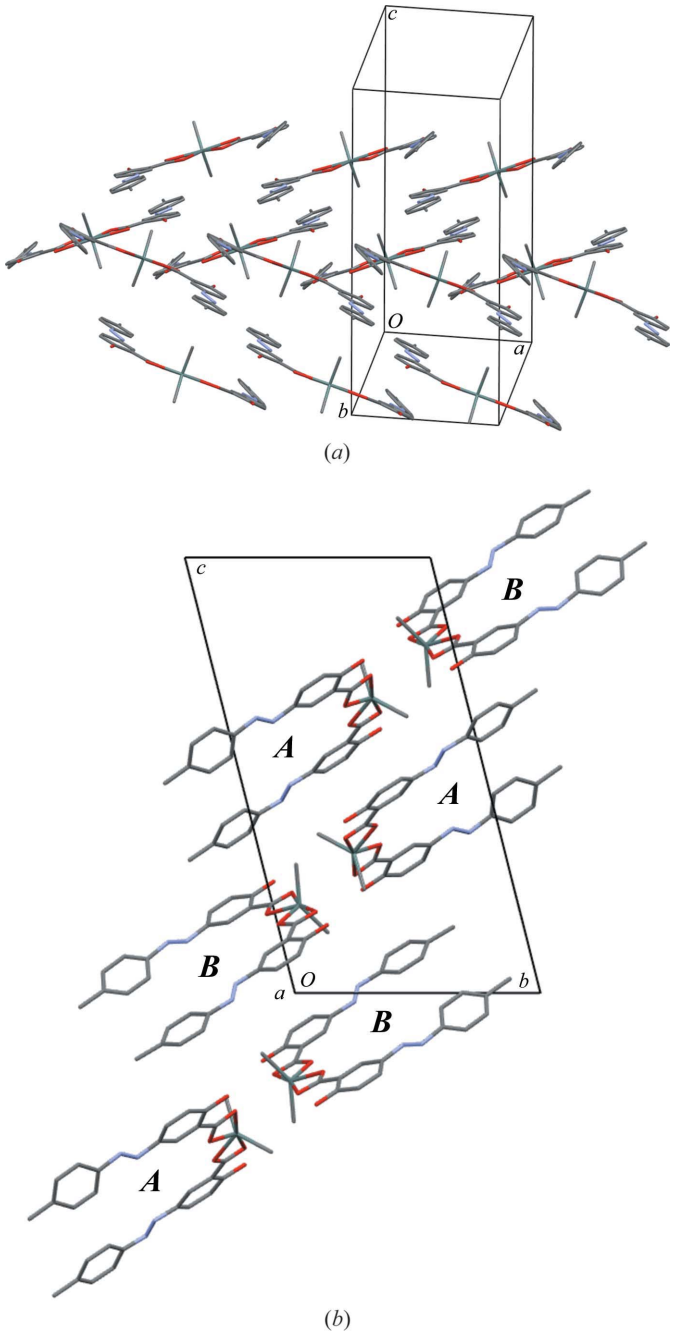


Figure 6
(*a*) The double-chains of *A* molecules of (I) (upper half of the image) and the differently tilted *B* molecules in the pairs of single chains (lower half of the image). Note the offset between the two *B* chains which precludes the 'stack of four' motif seen for the carboxylate ligands of the *A* molecules. (*b*) The alternating stacking along the [01$\bar{1}$] direction of chains of *A* and *B* molecules, showing the hydrophilic ends of the carboxylate ligands facing towards the centre of the ribbon-like layers. The chains are viewed end-on and H atoms have been omitted for clarity.

sides of the molecules in two such offset dimers also have weak π–π interactions ($Cg2\cdots Cg8^{vi}$; Table 7), which link the dimers into extended chains running parallel to the [100] direction (Fig. 7*b*), as represented by the combination of the black and red motifs in the cartoon in Fig. 4(*e*). Essentially, the relationship between adjacent dimers connected in this way is such they are shifted sideways so that the 'left-hand' pair of tolyl rings in the dimer is directly above the 'right-hand' pair in the next dimer, thereby forming a step-like pattern (Fig. 7*c*). The planes of the carboxylate ligands are slanted with respect to the chain direction. These interactions result once again in a short stack of four π–π-interacting tolyl rings involving all of the symmetry-unique tolyl rings from four molecules in two dimers in the sequence $Cg4\cdots Cg8\cdots Cg2\cdots Cg6$ (the relevant symmetry codes have been omitted from the given sequence designation for clarity, but these are given in Table 7). The stacks are finite because they are capped on each end by C34*A*—H$\cdots\pi$ and C70—H$\cdots\pi$ interactions involving *n*-butyl ligands of molecules in adjacent chains (Table 6). The motif in these chains differs from that found in (IV), because instead of the first two molecules in the short stack having their carboxylate ligand arms pointing in the same direction and opposite to that of the other two, the arms point in alternating directions as one progresses along the stack (Fig. 7*d*).

In addition to the above pattern, the two 2-hydroxyphenyl rings in molecule *A* (*Cg*1 and *Cg*3), together with the solvent benzene molecule (*Cg*9), form finite stacks of six rings from six molecules in the sequence $Cg9\cdots Cg3\cdots Cg1\cdots Cg1\cdots Cg3\cdots Cg9$ distributed about the centre of inversion at $(0, \frac{1}{2}, 0)$, although the $Cg1\cdots Cg1$ distance is rather long and the rings are quite offset (Table 7, and Figs. 8*a* and 8*b*). The junctions between the black, red and blue red motifs in Fig. 4(*e*) represent this. The stack is capped at each end by two symmetry-related C74*A*/*B*—H$\cdots\pi$ interactions involving molecule *B* *n*-butyl groups (Table 6). In this way, although the solvent molecule sits within the cavity formed by the above-described dimers, it is part of a stack from an offset group of molecules and is thus intricately involved in the supramolecular π–π interactions and makes a relevant contribution to the construction of the structure. The 2-hydroxyphenyl rings of molecule *B* (*Cg*5 and *Cg*7) form similar stacks of four rings from four molecules in the sequence $Cg7\cdots Cg5\cdots Cg5\cdots Cg7$ distributed about the centre of inversion at $(1, \frac{1}{2}, \frac{1}{2})$. Again the interactions are weak and the ring centroids are quite offset. The junctions between the black, red and magenta motifs in Fig. 4(*e*) represent this. The stack is capped at each end by two symmetry-related C30—H$\cdots\pi$ interactions involving molecule *A* *n*-butyl groups. Similar to the chains formed by the repeated stacks of tolyl rings, the interactions between the 2-hydroxyphenyl rings link molecules into pairs and then through sideways offsets relating each pair with the next one into chains of tilted molecules which extend parallel to [100] (Fig. 8*a*).

There are two main differences between the arrangements involving the tolyl rings and those involving the 2-hydroxyphenyl rings of (II). While the π–π interactions involving the tolyl rings link *A* and *B* molecules tail-to-tail into dimers (the tolyl groups are considered as tails here), and these *AB* dimers are linked into chains, the π–π interactions involving the 2-hydroxyphenyl rings link molecules head-to-head (the carboxylate ends of the molecules) into either *AA* or *BB* pairs and then side-to-side offset pairs are linked into chains of pure *A* or pure *B* molecules (Fig. 8*a*). Again, these chains of tilted

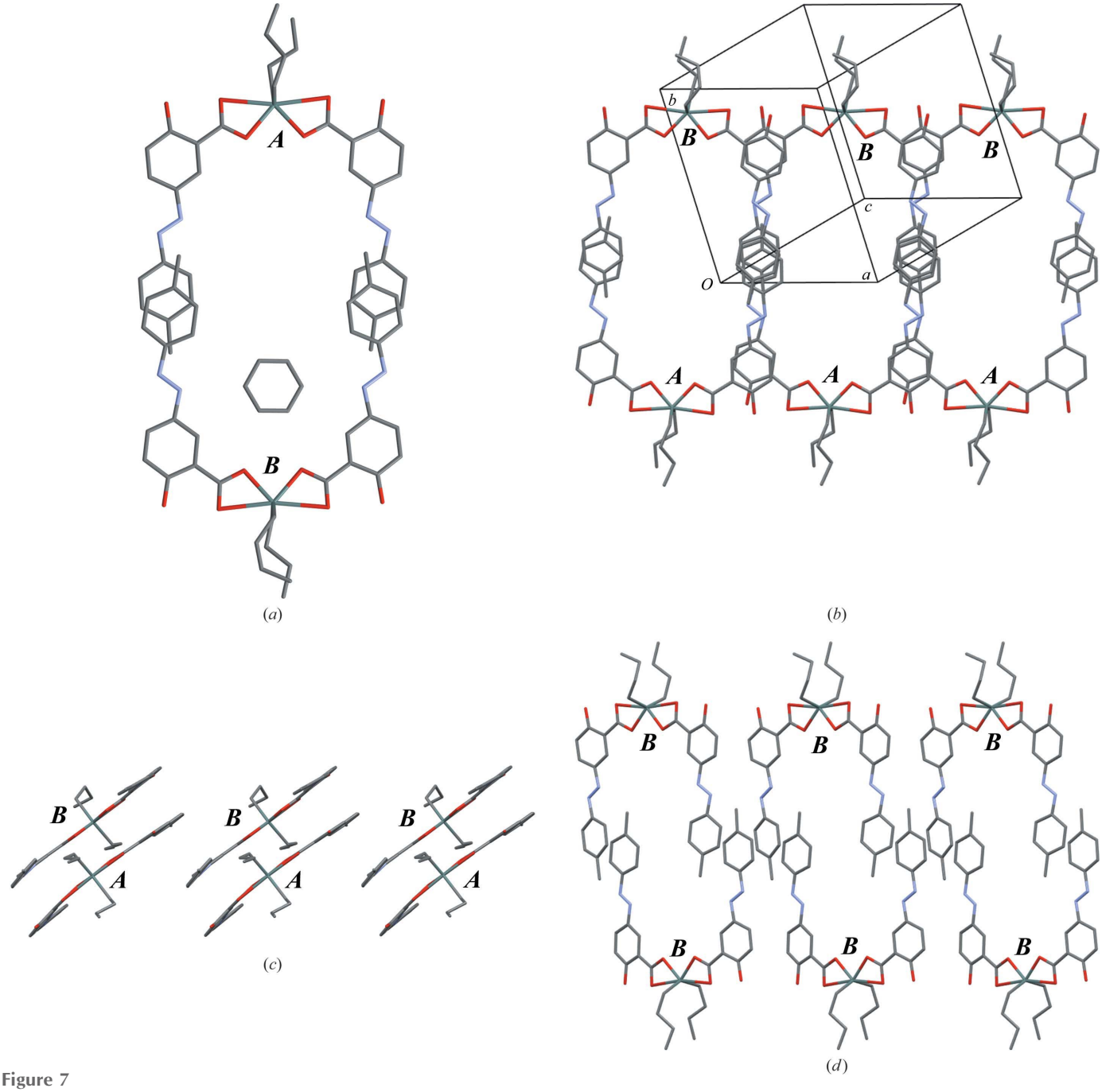


Figure 7
The building of the π–π stacking in (II), showing (*a*) dimer formation through tolyl–tolyl interactions between an *A* and a *B* molecule; (*b*) the linking of the dimers into chains *via* interactions between the 2-hydroxyphenyl rings of adjacent molecules; (*c*) a side view of the arrangement in (*b*) showing the step-like chains; (*d*) a rotation of the image in (*b*) showing the stack of four tolyl rings. H atoms have been omitted for clarity.

molecules run parallel to [100]. Since the tolyl groups of head-to-head groups of molecules form their own stacks, they thereby link adjacent chains of head-to-head molecules in the [012] direction, thus giving thick two-dimensional sheets of molecules, which lie parallel to the (012) plane [Figs. 4*e* (overall) and 8*b*]. The combination of these sheets with the stack-capping C—H$\cdots\pi$ interactions yields the complete three-dimensional supramolecular framework.

The crystal structures of a further seven related dialkylbis{5-[(*E*)-2-aryldiazen-1-yl]-2-hydroxybenzoato}tin(IV) complexes have been reported. Five of these display the single-chain motif depicted in Fig. 4(*b*). These involve alkyl = *n*-octyl and aryl = phenyl (Basu Baul *et al.*, 2007), alkyl = *n*-butyl and aryl = 4-chloro (Basu Baul *et al.*, 2003), and two di-*n*-butyl- and one dimethyltin(IV) complex in which the carboxylate ligands have different 4-substituted aryl groups (Basu Baul *et al.*, 2005). The final two structures are di-*n*-butyltin(IV) complexes with 2-methoxyphenyl and 2-methylphenyl aryl groups in the carboxylate ligands (Linden *et al.*, 2007; Basu Baul, Dhar & Tiekink, 2001). Steric effects from the 2-substitution

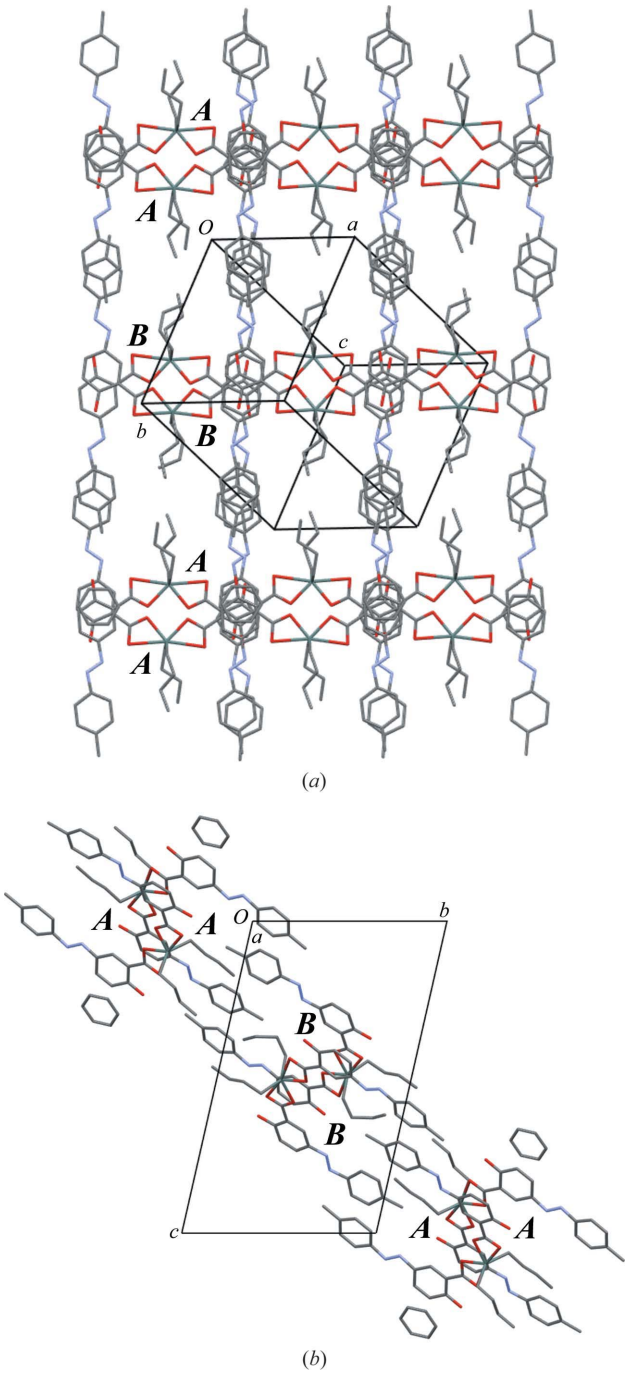


Figure 8
The two-dimensional layers formed by all π–π interactions in (II), showing (*a*) a view perpendicular to the layer and (*b*) a side view of a single layer showing its thickness. The lines of Sn^{IV} atoms and carboxylate groups near the top and bottom of the image contain Sn1 only (all *A* molecules) and the stacks including the solvent benzene molecules, while the line of Sn^{IV} atoms and carboxylate groups near the middle of the image contains Sn2 only (all *B* molecules) and no benzene molecules. H atoms have been omitted for clarity.

twist the plane of the terminal aryl group severely out of the plane of the remainder of the ligand for one of the carboxylate ligands and leads to more complicated stacking. In the former case, the chain motif shown in Fig. 4(*b*) may be discerned once again, where the 2-hydroxyphenyl rings of adjacent molecules are the main interacting species. In the latter case, the double-chain motif shown in Fig. 4(*f*) is present, which is part of the more complex motif depicted in Fig. 4(*e*). Again, the terminal aryl groups are not involved in any significant π–π stacking interactions.

There is only one other reported structure of a mononuclear discrete metal complex with two carboxylate ligands of the type discussed here. The diaquabis[2-hydroxy-5-(phenyldiazenyl)benzoato]zinc(II) complex (Jin *et al.*, 2015) has the carboxylate ligands in two quite different planes, thereby precluding the sorts of π–π stacking motifs described above, and indeed the structure contains no π–π interactions at all involving the carboxylate ligands.

In conclusion, the molecular structures of two new dialkylbis{5-[(*E*)-2-aryldiazen-1-yl]-2-hydroxybenzoato}tin(IV) complexes, (I) and (II), exhibit the usual skew-trapezoidal bipyramidal coordination geometry observed for related complexes of this class. The two extended planar carboxylate ligands in such complexes proffer the opportunity for π–π stacking interactions and all six complexes examined here display intriguing motifs for the overlay of the ligand from neighbouring molecules. While there are some recurring basic motifs amongst the observed stacking arrangements, such as dimers and step-like chains [structures (V) and (III)/(VI), respectively], variations through longitudinal slipping, which produces part of the pattern in (II) from (V), and/or inversion of the direction of the overlay, which produces (IV) and one of the motifs in (I) from (III), add complexity. The π–π stacking motifs in (I) and (II) are combinations of some of those observed in the other structures and are the most complex of the six structures examined. Curiously, it appears that the presence of two symmetry-independent Sn^{IV} complex molecules in both (I) and (II), which does not occur in the other four structures, is correlated with the complexity of the packing motifs.

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π–π stacking motifs in dialkylbis{5-[(*E*)-2-aryldiazen-1-yl]-2-hydroxybenzoato}tin(IV) complexes

Anthony Linden and Tushar S. Basu Baul

Computing details

For both compounds, data collection: *COLLECT* (Nonius, 2000); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL2014* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

(I) Dimethylbis{2-hydroxy-5-[(*E*)-2-(4-methylphenyl)diazen-1-\ yl]benzoato}tin(IV)

Crystal data

$[Sn(CH_3)_2(C_{14}H_{11}N_2O_3)_2]$
M_r = 659.25
Triclinic, $P\overline{1}$
a = 10.1883 (1) Å
b = 12.9209 (1) Å
c = 23.0447 (2) Å
α = 102.3524 (4)°
β = 95.2584 (4)°
γ = 104.1530 (5)°
V = 2840.09 (4) Å^3
Z = 4
$F(000)$ = 1336
D_x = 1.541 Mg m^{-3}
Melting point: 496 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 77568 reflections
θ = 2.0–30.0°
μ = 0.95 mm^{-1}
T = 160 K
Prism, yellow
0.30 × 0.20 × 0.11 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: Nonius FR590 sealed tube generator
Horizontally mounted graphite crystal monochromator
Detector resolution: 9 pixels mm^{-1}
φ and ω scans with κ offsets
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.805, T_{max} = 0.912
69932 measured reflections
16590 independent reflections
10414 reflections with $I > 2\sigma(I)$
R_{int} = 0.070
θ_{max} = 30.0°, θ_{min} = 2.1°
h = −14→14
k = −18→18
l = −32→32

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.099
S = 1.00
16590 reflections
763 parameters
0 restraints
Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0441P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.65$ e Å^{-3}
$\Delta\rho_{min} = -1.07$ e Å^{-3}

Special details

Experimental. Solvent used: benzene Cooling Device: Oxford Cryosystems Cryostream 700 Crystal mount: glued on a glass fibre Mosaicity (°.): 0.503 (1) Frames collected: 758 Seconds exposure per frame: 15 Degrees rotation per frame: 1.0 Crystal-Detector distance (mm): 33.4

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.10136 (2)	0.38257 (2)	0.32223 (2)	0.02512 (6)
O1	0.25573 (18)	0.50245 (15)	0.38461 (8)	0.0285 (4)
O2	0.34413 (19)	0.36401 (16)	0.35559 (9)	0.0337 (5)
O3	0.5996 (2)	0.38169 (18)	0.39426 (10)	0.0363 (5)
H3	0.521 (4)	0.353 (4)	0.3804 (19)	0.094 (17)*
O4	−0.00723 (19)	0.50043 (15)	0.34064 (8)	0.0311 (5)
O5	−0.14973 (19)	0.36505 (15)	0.27117 (9)	0.0314 (5)
O6	−0.3961 (2)	0.38172 (17)	0.23716 (9)	0.0336 (5)
H6	−0.344 (3)	0.350 (3)	0.2374 (16)	0.052 (12)*
N1	0.6293 (2)	0.8055 (2)	0.52231 (10)	0.0304 (6)
N2	0.7395 (2)	0.85626 (19)	0.55732 (10)	0.0304 (6)
N3	−0.2189 (2)	0.81187 (18)	0.37749 (10)	0.0266 (5)
N4	−0.2911 (2)	0.87516 (19)	0.36858 (10)	0.0293 (5)
C1	0.3583 (3)	0.4601 (2)	0.38642 (12)	0.0263 (6)
C2	0.4893 (3)	0.5268 (2)	0.42365 (12)	0.0239 (6)
C3	0.6026 (3)	0.4841 (2)	0.42542 (12)	0.0272 (6)
C4	0.7282 (3)	0.5489 (2)	0.45927 (13)	0.0308 (7)
H4	0.8056	0.5202	0.4599	0.037*
C5	0.7396 (3)	0.6539 (2)	0.49150 (12)	0.0292 (7)
H5	0.8249	0.6974	0.5146	0.035*
C6	0.6270 (3)	0.6975 (2)	0.49066 (12)	0.0262 (6)
C7	0.5031 (3)	0.6339 (2)	0.45627 (12)	0.0273 (6)
H7	0.4268	0.6638	0.4550	0.033*
C8	0.7434 (3)	0.9646 (2)	0.58893 (12)	0.0281 (6)
C9	0.6412 (3)	1.0163 (3)	0.58016 (14)	0.0378 (8)
H9	0.5625	0.9795	0.5508	0.045*
C10	0.6540 (3)	1.1212 (3)	0.61410 (14)	0.0399 (8)
H10	0.5831	1.1556	0.6082	0.048*
C11	0.7696 (3)	1.1776 (2)	0.65696 (13)	0.0344 (7)
C12	0.8729 (3)	1.1262 (2)	0.66414 (13)	0.0349 (7)
H12	0.9531	1.1637	0.6925	0.042*
C13	0.8601 (3)	1.0205 (2)	0.63025 (13)	0.0328 (7)

H13	0.9316	0.9864	0.6354	0.039*
C14	−0.1235 (3)	0.4599 (2)	0.30469 (12)	0.0272 (6)
C15	−0.2184 (3)	0.5285 (2)	0.30485 (12)	0.0247 (6)
C16	−0.3503 (3)	0.4863 (2)	0.27060 (12)	0.0266 (6)
C17	−0.4382 (3)	0.5535 (2)	0.27123 (13)	0.0296 (7)
H17	−0.5267	0.5252	0.2478	0.035*
C18	−0.3987 (3)	0.6600 (2)	0.30525 (12)	0.0282 (6)
H18	−0.4602	0.7046	0.3055	0.034*
C19	−0.2681 (3)	0.7035 (2)	0.33971 (12)	0.0249 (6)
C20	−0.1805 (3)	0.6370 (2)	0.33952 (12)	0.0252 (6)
H20	−0.0927	0.6656	0.3635	0.030*
C21	−0.2457 (3)	0.9831 (2)	0.40756 (12)	0.0257 (6)
C22	−0.1456 (3)	1.0157 (2)	0.45712 (13)	0.0365 (7)
H22	−0.0990	0.9651	0.4670	0.044*
C23	−0.1129 (3)	1.1218 (2)	0.49247 (13)	0.0379 (8)
H23	−0.0435	1.1432	0.5266	0.045*
C24	−0.1792 (3)	1.1978 (2)	0.47928 (13)	0.0290 (6)
C25	−0.2793 (3)	1.1641 (2)	0.42959 (15)	0.0398 (8)
H25	−0.3264	1.2146	0.4198	0.048*
C26	−0.3126 (3)	1.0579 (2)	0.39364 (14)	0.0373 (8)
H26	−0.3815	1.0364	0.3594	0.045*
C27	0.7830 (3)	1.2919 (3)	0.69461 (15)	0.0473 (9)
H271	0.7147	1.2884	0.7219	0.071*
H272	0.7679	1.3395	0.6682	0.071*
H273	0.8750	1.3219	0.7180	0.071*
C28	−0.1414 (3)	1.3135 (2)	0.51864 (14)	0.0372 (8)
H281	−0.2028	1.3539	0.5047	0.056*
H282	−0.0466	1.3509	0.5164	0.056*
H283	−0.1505	1.3108	0.5603	0.056*
C29	0.1619 (3)	0.3892 (3)	0.23862 (13)	0.0387 (8)
H291	0.1713	0.4634	0.2327	0.058*
H292	0.0927	0.3358	0.2068	0.058*
H293	0.2499	0.3716	0.2371	0.058*
C30	0.0148 (3)	0.2604 (2)	0.36471 (14)	0.0385 (8)
H301	−0.0138	0.2942	0.4020	0.058*
H302	0.0826	0.2218	0.3741	0.058*
H303	−0.0650	0.2079	0.3380	0.058*
Sn2	−0.60835 (2)	0.10939 (2)	0.20193 (2)	0.02463 (6)
O41	−0.50211 (18)	0.00346 (15)	0.15816 (8)	0.0288 (4)
O42	−0.35771 (19)	0.16857 (15)	0.18648 (9)	0.0315 (5)
O43	−0.1099 (2)	0.20069 (18)	0.15594 (11)	0.0387 (6)
H43	−0.162 (4)	0.214 (3)	0.1736 (16)	0.054 (13)*
O44	−0.77008 (19)	−0.03372 (15)	0.18092 (9)	0.0319 (5)
O45	−0.86084 (19)	0.09139 (16)	0.23033 (8)	0.0323 (5)
O46	−1.1085 (2)	0.02763 (18)	0.25580 (10)	0.0376 (5)
H46	−1.038 (3)	0.073 (3)	0.2515 (15)	0.051 (11)*
N41	−0.2835 (2)	−0.23287 (19)	0.02011 (10)	0.0292 (5)
N42	−0.2053 (2)	−0.2628 (2)	−0.01555 (10)	0.0306 (6)

N43	−1.1311 (2)	−0.3884 (2)	0.11860 (11)	0.0314 (6)
N44	−1.2365 (2)	−0.4641 (2)	0.11707 (10)	0.0313 (6)
C41	−0.3834 (3)	0.0701 (2)	0.15825 (12)	0.0265 (6)
C42	−0.2859 (3)	0.0273 (2)	0.12326 (12)	0.0247 (6)
C43	−0.1556 (3)	0.0956 (2)	0.12328 (13)	0.0287 (6)
C44	−0.0657 (3)	0.0551 (2)	0.08834 (13)	0.0318 (7)
H44	0.0222	0.1014	0.0880	0.038*
C45	−0.1047 (3)	−0.0524 (2)	0.05437 (13)	0.0305 (7)
H45	−0.0428	−0.0798	0.0310	0.037*
C46	−0.2346 (3)	−0.1215 (2)	0.05404 (12)	0.0269 (6)
C47	−0.3226 (3)	−0.0808 (2)	0.08837 (12)	0.0269 (6)
H47	−0.4106	−0.1274	0.0883	0.032*
C48	−0.2533 (3)	−0.3745 (2)	−0.04892 (12)	0.0281 (6)
C49	−0.3806 (3)	−0.4456 (2)	−0.04775 (13)	0.0353 (7)
H49	−0.4426	−0.4196	−0.0239	0.042*
C50	−0.4164 (3)	−0.5536 (3)	−0.08129 (13)	0.0383 (8)
H50	−0.5030	−0.6013	−0.0802	0.046*
C51	−0.3265 (3)	−0.5931 (2)	−0.11675 (13)	0.0320 (7)
C52	−0.2020 (3)	−0.5218 (3)	−0.11793 (13)	0.0352 (7)
H52	−0.1397	−0.5479	−0.1416	0.042*
C53	−0.1657 (3)	−0.4131 (3)	−0.08544 (13)	0.0332 (7)
H53	−0.0809	−0.3648	−0.0881	0.040*
C54	−0.8724 (3)	−0.0069 (2)	0.20316 (12)	0.0294 (6)
C55	−1.0001 (3)	−0.0942 (2)	0.19579 (12)	0.0260 (6)
C56	−1.1115 (3)	−0.0731 (2)	0.22349 (12)	0.0275 (6)
C57	−1.2287 (3)	−0.1595 (2)	0.21874 (12)	0.0310 (7)
H57	−1.3026	−0.1460	0.2388	0.037*
C58	−1.2383 (3)	−0.2631 (2)	0.18551 (13)	0.0306 (7)
H58	−1.3189	−0.3208	0.1824	0.037*
C59	−1.1297 (3)	−0.2847 (2)	0.15587 (12)	0.0272 (6)
C60	−1.0120 (3)	−0.2002 (2)	0.16222 (12)	0.0284 (6)
H60	−0.9373	−0.2149	0.1432	0.034*
C61	−1.2412 (3)	−0.5668 (2)	0.07783 (12)	0.0281 (6)
C62	−1.1566 (3)	−0.5803 (3)	0.03444 (13)	0.0368 (7)
H62	−1.0901	−0.5184	0.0293	0.044*
C63	−1.1693 (3)	−0.6832 (3)	−0.00090 (13)	0.0386 (8)
H63	−1.1111	−0.6916	−0.0305	0.046*
C64	−1.2655 (3)	−0.7757 (2)	0.00558 (13)	0.0328 (7)
C65	−1.3511 (3)	−0.7603 (3)	0.04800 (14)	0.0396 (8)
H65	−1.4193	−0.8218	0.0524	0.047*
C66	−1.3393 (3)	−0.6569 (2)	0.08424 (14)	0.0367 (7)
H66	−1.3984	−0.6480	0.1134	0.044*
C67	−0.3666 (3)	−0.7128 (3)	−0.15153 (14)	0.0426 (8)
H671	−0.4312	−0.7226	−0.1878	0.064*
H672	−0.4099	−0.7593	−0.1263	0.064*
H673	−0.2847	−0.7338	−0.1630	0.064*
C68	−1.2762 (3)	−0.8892 (3)	−0.03241 (13)	0.0428 (8)
H681	−1.2550	−0.8838	−0.0725	0.064*

H682	−1.3695	−0.9362	−0.0360	0.064*
H683	−1.2111	−0.9211	−0.0134	0.064*
C69	−0.5492 (3)	0.1368 (3)	0.29454 (12)	0.0376 (8)
H691	−0.6033	0.1807	0.3163	0.056*
H692	−0.4518	0.1764	0.3052	0.056*
H693	−0.5647	0.0660	0.3055	0.056*
C70	−0.6591 (3)	0.1953 (2)	0.13960 (13)	0.0330 (7)
H701	−0.6566	0.1540	0.0989	0.049*
H702	−0.5931	0.2680	0.1482	0.049*
H703	−0.7513	0.2041	0.1425	0.049*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.02441 (11)	0.02026 (11)	0.02735 (11)	0.00554 (8)	0.00105 (8)	0.00053 (8)
O1	0.0234 (10)	0.0262 (11)	0.0306 (11)	0.0066 (9)	−0.0030 (8)	−0.0010 (8)
O2	0.0301 (11)	0.0228 (11)	0.0426 (12)	0.0067 (9)	0.0002 (9)	−0.0009 (9)
O3	0.0316 (13)	0.0246 (12)	0.0501 (14)	0.0115 (10)	0.0009 (10)	0.0016 (10)
O4	0.0254 (11)	0.0260 (11)	0.0372 (12)	0.0095 (9)	−0.0035 (9)	−0.0017 (9)
O5	0.0296 (11)	0.0233 (11)	0.0359 (12)	0.0083 (9)	−0.0002 (9)	−0.0032 (9)
O6	0.0261 (12)	0.0244 (12)	0.0407 (13)	0.0030 (10)	−0.0044 (9)	−0.0039 (9)
N1	0.0265 (13)	0.0288 (14)	0.0313 (13)	0.0045 (11)	0.0021 (10)	0.0021 (11)
N2	0.0287 (13)	0.0272 (14)	0.0319 (14)	0.0046 (11)	0.0008 (11)	0.0047 (11)
N3	0.0264 (13)	0.0214 (13)	0.0307 (13)	0.0071 (10)	0.0022 (10)	0.0039 (10)
N4	0.0297 (13)	0.0247 (13)	0.0337 (14)	0.0082 (11)	0.0055 (10)	0.0063 (11)
C1	0.0254 (15)	0.0254 (16)	0.0266 (15)	0.0051 (12)	0.0031 (12)	0.0055 (12)
C2	0.0224 (14)	0.0252 (15)	0.0246 (14)	0.0062 (12)	0.0024 (11)	0.0079 (12)
C3	0.0314 (16)	0.0259 (16)	0.0269 (15)	0.0101 (13)	0.0060 (12)	0.0085 (12)
C4	0.0239 (15)	0.0325 (17)	0.0372 (17)	0.0102 (13)	0.0013 (12)	0.0097 (14)
C5	0.0212 (15)	0.0333 (17)	0.0312 (16)	0.0050 (13)	−0.0001 (12)	0.0079 (13)
C6	0.0266 (15)	0.0264 (16)	0.0243 (14)	0.0058 (12)	0.0039 (11)	0.0052 (12)
C7	0.0276 (15)	0.0254 (16)	0.0282 (15)	0.0087 (13)	0.0040 (12)	0.0033 (12)
C8	0.0298 (16)	0.0250 (16)	0.0273 (15)	0.0036 (13)	0.0036 (12)	0.0062 (12)
C9	0.0306 (17)	0.0355 (19)	0.0417 (19)	0.0053 (14)	−0.0001 (14)	0.0046 (15)
C10	0.0354 (18)	0.0325 (18)	0.051 (2)	0.0106 (15)	0.0091 (15)	0.0071 (15)
C11	0.0419 (19)	0.0252 (17)	0.0328 (17)	0.0017 (14)	0.0129 (14)	0.0055 (13)
C12	0.0378 (18)	0.0304 (18)	0.0309 (16)	−0.0007 (14)	−0.0004 (13)	0.0095 (13)
C13	0.0333 (17)	0.0253 (16)	0.0360 (17)	0.0027 (13)	0.0003 (13)	0.0077 (13)
C14	0.0264 (15)	0.0240 (16)	0.0284 (15)	0.0059 (12)	0.0027 (12)	0.0021 (12)
C15	0.0261 (15)	0.0236 (15)	0.0229 (14)	0.0053 (12)	0.0030 (11)	0.0047 (11)
C16	0.0277 (15)	0.0263 (16)	0.0224 (14)	0.0033 (13)	0.0016 (11)	0.0038 (12)
C17	0.0203 (14)	0.0301 (17)	0.0342 (16)	0.0031 (13)	0.0005 (12)	0.0050 (13)
C18	0.0244 (15)	0.0276 (16)	0.0338 (16)	0.0091 (13)	0.0040 (12)	0.0077 (13)
C19	0.0239 (14)	0.0216 (15)	0.0273 (15)	0.0033 (12)	0.0025 (11)	0.0060 (12)
C20	0.0220 (14)	0.0266 (16)	0.0260 (15)	0.0067 (12)	0.0005 (11)	0.0054 (12)
C21	0.0257 (15)	0.0236 (15)	0.0285 (15)	0.0083 (12)	0.0060 (12)	0.0051 (12)
C22	0.0438 (19)	0.0282 (17)	0.0385 (18)	0.0182 (15)	−0.0039 (14)	0.0045 (14)
C23	0.046 (2)	0.0337 (18)	0.0327 (17)	0.0169 (16)	−0.0036 (14)	0.0022 (14)

C24	0.0275 (16)	0.0263 (16)	0.0350 (16)	0.0085 (13)	0.0113 (13)	0.0073 (13)
C25	0.0376 (18)	0.0252 (17)	0.059 (2)	0.0165 (15)	−0.0045 (16)	0.0104 (15)
C26	0.0335 (17)	0.0300 (18)	0.0449 (19)	0.0109 (14)	−0.0120 (14)	0.0065 (14)
C27	0.056 (2)	0.0306 (19)	0.050 (2)	0.0054 (17)	0.0137 (17)	0.0038 (16)
C28	0.0387 (18)	0.0283 (17)	0.0425 (19)	0.0126 (15)	0.0060 (14)	0.0002 (14)
C29	0.0324 (17)	0.045 (2)	0.0311 (17)	−0.0008 (15)	0.0072 (13)	0.0050 (15)
C30	0.0430 (19)	0.0277 (17)	0.0409 (19)	0.0022 (15)	0.0030 (15)	0.0100 (14)
Sn2	0.02260 (11)	0.02230 (11)	0.02507 (11)	0.00392 (8)	0.00101 (8)	0.00108 (8)
O41	0.0215 (10)	0.0234 (11)	0.0358 (11)	0.0027 (8)	0.0050 (8)	−0.0012 (9)
O42	0.0274 (11)	0.0230 (11)	0.0370 (12)	0.0042 (9)	0.0034 (9)	−0.0043 (9)
O43	0.0268 (12)	0.0280 (13)	0.0500 (15)	−0.0013 (10)	0.0048 (11)	−0.0035 (10)
O44	0.0265 (11)	0.0259 (11)	0.0357 (12)	−0.0010 (9)	0.0071 (9)	−0.0004 (9)
O45	0.0304 (11)	0.0260 (11)	0.0339 (11)	0.0018 (9)	0.0026 (9)	0.0012 (9)
O46	0.0378 (13)	0.0275 (13)	0.0409 (13)	0.0030 (11)	0.0115 (10)	−0.0010 (10)
N41	0.0281 (13)	0.0256 (14)	0.0338 (14)	0.0080 (11)	0.0049 (11)	0.0062 (11)
N42	0.0330 (14)	0.0310 (14)	0.0302 (13)	0.0128 (12)	0.0042 (11)	0.0078 (11)
N43	0.0280 (13)	0.0286 (14)	0.0340 (14)	0.0031 (11)	0.0069 (11)	0.0045 (11)
N44	0.0298 (14)	0.0272 (14)	0.0346 (14)	0.0039 (11)	0.0069 (11)	0.0066 (11)
C41	0.0236 (15)	0.0242 (16)	0.0277 (15)	0.0045 (12)	−0.0021 (11)	0.0027 (12)
C42	0.0197 (14)	0.0249 (15)	0.0267 (15)	0.0035 (12)	0.0011 (11)	0.0046 (12)
C43	0.0232 (15)	0.0257 (16)	0.0333 (16)	0.0035 (12)	−0.0026 (12)	0.0058 (13)
C44	0.0202 (15)	0.0352 (18)	0.0359 (17)	0.0013 (13)	0.0021 (12)	0.0085 (14)
C45	0.0251 (15)	0.0369 (18)	0.0333 (16)	0.0133 (14)	0.0058 (12)	0.0102 (14)
C46	0.0268 (15)	0.0265 (16)	0.0262 (15)	0.0056 (13)	0.0028 (12)	0.0062 (12)
C47	0.0229 (14)	0.0279 (16)	0.0281 (15)	0.0040 (12)	0.0011 (11)	0.0076 (12)
C48	0.0304 (16)	0.0280 (16)	0.0268 (15)	0.0102 (13)	0.0019 (12)	0.0070 (12)
C49	0.0322 (17)	0.0362 (19)	0.0354 (17)	0.0106 (14)	0.0098 (13)	0.0007 (14)
C50	0.0310 (17)	0.0387 (19)	0.0390 (18)	0.0050 (15)	0.0026 (14)	0.0024 (15)
C51	0.0370 (17)	0.0314 (17)	0.0280 (16)	0.0113 (14)	0.0023 (13)	0.0066 (13)
C52	0.0429 (19)	0.0358 (19)	0.0316 (17)	0.0180 (16)	0.0131 (14)	0.0067 (14)
C53	0.0311 (16)	0.0372 (18)	0.0326 (16)	0.0095 (14)	0.0076 (13)	0.0099 (14)
C54	0.0310 (16)	0.0295 (17)	0.0237 (15)	0.0033 (13)	0.0018 (12)	0.0050 (12)
C55	0.0227 (14)	0.0275 (16)	0.0245 (14)	0.0037 (12)	0.0025 (11)	0.0039 (12)
C56	0.0299 (16)	0.0266 (16)	0.0235 (14)	0.0065 (13)	0.0007 (12)	0.0037 (12)
C57	0.0254 (15)	0.0347 (18)	0.0307 (16)	0.0047 (13)	0.0084 (12)	0.0057 (13)
C58	0.0260 (15)	0.0291 (17)	0.0340 (16)	0.0017 (13)	0.0071 (12)	0.0075 (13)
C59	0.0255 (15)	0.0254 (16)	0.0308 (16)	0.0059 (12)	0.0060 (12)	0.0073 (12)
C60	0.0253 (15)	0.0325 (17)	0.0262 (15)	0.0055 (13)	0.0056 (12)	0.0065 (12)
C61	0.0261 (15)	0.0258 (16)	0.0316 (16)	0.0056 (13)	0.0046 (12)	0.0071 (13)
C62	0.0297 (17)	0.0408 (19)	0.0359 (17)	0.0024 (14)	0.0090 (13)	0.0075 (15)
C63	0.0341 (18)	0.046 (2)	0.0307 (17)	0.0077 (16)	0.0085 (13)	0.0004 (15)
C64	0.0344 (17)	0.0338 (18)	0.0270 (16)	0.0109 (14)	−0.0028 (13)	0.0017 (13)
C65	0.0434 (19)	0.0279 (18)	0.0436 (19)	0.0027 (15)	0.0069 (15)	0.0085 (15)
C66	0.0416 (19)	0.0303 (18)	0.0372 (18)	0.0058 (15)	0.0159 (14)	0.0061 (14)
C67	0.051 (2)	0.037 (2)	0.0388 (19)	0.0152 (16)	0.0123 (15)	0.0007 (15)
C68	0.052 (2)	0.040 (2)	0.0330 (18)	0.0188 (17)	−0.0033 (15)	−0.0020 (15)
C69	0.0452 (19)	0.0366 (19)	0.0267 (16)	0.0110 (15)	−0.0026 (14)	0.0020 (14)
C70	0.0264 (16)	0.0391 (19)	0.0338 (17)	0.0063 (14)	0.0009 (13)	0.0141 (14)

Geometric parameters (Å, º)

Sn1—O1	2.0930 (17)	Sn2—O41	2.0966 (17)
Sn1—O2	2.6051 (18)	Sn2—O42	2.5613 (19)
Sn1—O4	2.0872 (17)	Sn2—O44	2.0855 (19)
Sn1—O5	2.6517 (18)	Sn2—O45	2.6798 (19)
Sn1—C29	2.089 (3)	Sn2—C69	2.093 (3)
Sn1—C30	2.090 (3)	Sn2—C70	2.095 (3)
O1—C1	1.294 (3)	O41—C41	1.302 (3)
O2—C1	1.258 (3)	O42—C41	1.250 (3)
O3—C3	1.355 (3)	O43—C43	1.348 (3)
O3—H3	0.80 (4)	O43—H43	0.72 (3)
O4—C14	1.302 (3)	O44—C54	1.292 (3)
O5—C14	1.251 (3)	O45—C54	1.261 (3)
O6—C16	1.348 (3)	O46—C56	1.346 (3)
O6—H6	0.75 (3)	O46—H46	0.84 (3)
N1—N2	1.261 (3)	N41—N42	1.262 (3)
N1—C6	1.423 (3)	N41—C46	1.423 (3)
N2—C8	1.422 (3)	N42—C48	1.423 (3)
N3—N4	1.261 (3)	N43—N44	1.256 (3)
N3—C19	1.423 (3)	N43—C59	1.424 (3)
N4—C21	1.427 (3)	N44—C61	1.424 (3)
C1—C2	1.474 (4)	C41—C42	1.472 (4)
C2—C7	1.393 (4)	C42—C47	1.395 (4)
C2—C3	1.397 (4)	C42—C43	1.402 (4)
C3—C4	1.401 (4)	C43—C44	1.397 (4)
C4—C5	1.372 (4)	C44—C45	1.381 (4)
C4—H4	0.9500	C44—H44	0.9500
C5—C6	1.396 (4)	C45—C46	1.402 (4)
C5—H5	0.9500	C45—H45	0.9500
C6—C7	1.388 (4)	C46—C47	1.375 (4)
C7—H7	0.9500	C47—H47	0.9500
C8—C13	1.385 (4)	C48—C53	1.388 (4)
C8—C9	1.390 (4)	C48—C49	1.401 (4)
C9—C10	1.381 (4)	C49—C50	1.384 (4)
C9—H9	0.9500	C49—H49	0.9500
C10—C11	1.398 (4)	C50—C51	1.399 (4)
C10—H10	0.9500	C50—H50	0.9500
C11—C12	1.390 (4)	C51—C52	1.380 (4)
C11—C27	1.512 (4)	C51—C67	1.517 (4)
C12—C13	1.389 (4)	C52—C53	1.384 (4)
C12—H12	0.9500	C52—H52	0.9500
C13—H13	0.9500	C53—H53	0.9500
C14—C15	1.463 (4)	C54—C55	1.468 (4)
C15—C20	1.396 (4)	C55—C60	1.392 (4)
C15—C16	1.411 (4)	C55—C56	1.407 (4)
C16—C17	1.390 (4)	C56—C57	1.399 (4)
C17—C18	1.372 (4)	C57—C58	1.369 (4)

C17—H17	0.9500	C57—H57	0.9500
C18—C19	1.402 (4)	C58—C59	1.406 (4)
C18—H18	0.9500	C58—H58	0.9500
C19—C20	1.382 (4)	C59—C60	1.382 (4)
C20—H20	0.9500	C60—H60	0.9500
C21—C22	1.375 (4)	C61—C66	1.381 (4)
C21—C26	1.385 (4)	C61—C62	1.389 (4)
C22—C23	1.379 (4)	C62—C63	1.371 (4)
C22—H22	0.9500	C62—H62	0.9500
C23—C24	1.389 (4)	C63—C64	1.394 (4)
C23—H23	0.9500	C63—H63	0.9500
C24—C25	1.377 (4)	C64—C65	1.383 (4)
C24—C28	1.510 (4)	C64—C68	1.510 (4)
C25—C26	1.385 (4)	C65—C66	1.387 (4)
C25—H25	0.9500	C65—H65	0.9500
C26—H26	0.9500	C66—H66	0.9500
C27—H271	0.9800	C67—H671	0.9800
C27—H272	0.9800	C67—H672	0.9800
C27—H273	0.9800	C67—H673	0.9800
C28—H281	0.9800	C68—H681	0.9800
C28—H282	0.9800	C68—H682	0.9800
C28—H283	0.9800	C68—H683	0.9800
C29—H291	0.9800	C69—H691	0.9800
C29—H292	0.9800	C69—H692	0.9800
C29—H293	0.9800	C69—H693	0.9800
C30—H301	0.9800	C70—H701	0.9800
C30—H302	0.9800	C70—H702	0.9800
C30—H303	0.9800	C70—H703	0.9800

O1—Sn1—O4	82.93 (7)	O41—Sn2—O44	83.06 (7)
O1—Sn1—O5	136.76 (6)	O41—Sn2—O45	136.67 (7)
O1—Sn1—C29	104.91 (10)	O41—Sn2—C69	107.65 (10)
O1—Sn1—C30	107.95 (10)	O41—Sn2—C70	105.62 (10)
O2—Sn1—O4	137.49 (7)	O42—Sn2—O44	138.31 (6)
O2—Sn1—O5	168.41 (6)	O42—Sn2—O45	168.07 (6)
O2—Sn1—C29	86.97 (10)	O42—Sn2—C69	90.91 (10)
O2—Sn1—C30	89.97 (10)	O42—Sn2—C70	89.12 (9)
O4—Sn1—C29	105.62 (11)	O44—Sn2—C69	103.72 (11)
O4—Sn1—C30	105.34 (10)	O44—Sn2—C70	103.02 (10)
O5—Sn1—C29	86.87 (10)	O45—Sn2—C69	84.44 (10)
O5—Sn1—C30	87.83 (10)	O45—Sn2—C70	87.28 (9)
C29—Sn1—C30	136.93 (12)	C69—Sn2—C70	139.25 (12)
O1—Sn1—O2	54.57 (6)	O41—Sn2—O42	55.25 (6)
O4—Sn1—O5	53.89 (6)	O44—Sn2—O45	53.62 (6)
C1—O1—Sn1	104.55 (16)	C41—O41—Sn2	102.78 (16)
C1—O2—Sn1	81.64 (15)	C41—O42—Sn2	82.61 (16)
C3—O3—H3	105 (3)	C43—O43—H43	109 (3)
C14—O4—Sn1	105.80 (16)	C54—O44—Sn2	106.52 (17)

C14—O5—Sn1	80.75 (15)	C54—O45—Sn2	79.59 (16)
C16—O6—H6	113 (3)	C56—O46—H46	109 (2)
N2—N1—C6	113.8 (2)	N42—N41—C46	114.2 (2)
N1—N2—C8	114.3 (2)	N41—N42—C48	114.3 (2)
N4—N3—C19	113.9 (2)	N44—N43—C59	114.0 (2)
N3—N4—C21	114.5 (2)	N43—N44—C61	114.2 (2)
O2—C1—O1	119.2 (2)	O42—C41—O41	119.0 (2)
O2—C1—C2	121.9 (2)	O42—C41—C42	122.4 (3)
O1—C1—C2	118.9 (2)	O41—C41—C42	118.5 (2)
C7—C2—C3	119.1 (3)	C47—C42—C43	118.8 (3)
C7—C2—C1	120.7 (2)	C47—C42—C41	120.7 (2)
C3—C2—C1	120.2 (2)	C43—C42—C41	120.4 (2)
O3—C3—C2	123.2 (3)	O43—C43—C44	116.7 (3)
O3—C3—C4	116.7 (3)	O43—C43—C42	123.4 (3)
C2—C3—C4	120.1 (3)	C44—C43—C42	119.9 (3)
C5—C4—C3	120.0 (3)	C45—C44—C43	119.9 (3)
C5—C4—H4	120.0	C45—C44—H44	120.0
C3—C4—H4	120.0	C43—C44—H44	120.0
C4—C5—C6	120.6 (3)	C44—C45—C46	120.7 (3)
C4—C5—H5	119.7	C44—C45—H45	119.6
C6—C5—H5	119.7	C46—C45—H45	119.6
C7—C6—C5	119.4 (3)	C47—C46—C45	118.9 (3)
C7—C6—N1	116.1 (2)	C47—C46—N41	116.6 (2)
C5—C6—N1	124.6 (3)	C45—C46—N41	124.5 (3)
C6—C7—C2	120.8 (3)	C46—C47—C42	121.7 (3)
C6—C7—H7	119.6	C46—C47—H47	119.2
C2—C7—H7	119.6	C42—C47—H47	119.2
C13—C8—C9	119.6 (3)	C53—C48—C49	119.1 (3)
C13—C8—N2	115.8 (3)	C53—C48—N42	116.1 (3)
C9—C8—N2	124.6 (3)	C49—C48—N42	124.8 (3)
C10—C9—C8	120.0 (3)	C50—C49—C48	120.2 (3)
C10—C9—H9	120.0	C50—C49—H49	119.9
C8—C9—H9	120.0	C48—C49—H49	119.9
C9—C10—C11	121.1 (3)	C49—C50—C51	120.6 (3)
C9—C10—H10	119.5	C49—C50—H50	119.7
C11—C10—H10	119.5	C51—C50—H50	119.7
C12—C11—C10	118.4 (3)	C52—C51—C50	118.5 (3)
C12—C11—C27	120.5 (3)	C52—C51—C67	122.0 (3)
C10—C11—C27	121.1 (3)	C50—C51—C67	119.5 (3)
C13—C12—C11	120.6 (3)	C51—C52—C53	121.5 (3)
C13—C12—H12	119.7	C51—C52—H52	119.2
C11—C12—H12	119.7	C53—C52—H52	119.2
C8—C13—C12	120.3 (3)	C52—C53—C48	120.0 (3)
C8—C13—H13	119.9	C52—C53—H53	120.0
C12—C13—H13	119.9	C48—C53—H53	120.0
O5—C14—O4	119.5 (2)	O45—C54—O44	120.3 (3)
O5—C14—C15	122.5 (2)	O45—C54—C55	122.1 (3)
O4—C14—C15	118.0 (2)	O44—C54—C55	117.7 (2)

C20—C15—C16	118.7 (2)	C60—C55—C56	118.8 (3)
C20—C15—C14	120.6 (2)	C60—C55—C54	120.4 (3)
C16—C15—C14	120.8 (2)	C56—C55—C54	120.7 (2)
O6—C16—C17	117.9 (2)	O46—C56—C57	118.2 (3)
O6—C16—C15	122.4 (2)	O46—C56—C55	122.3 (3)
C17—C16—C15	119.6 (3)	C57—C56—C55	119.5 (3)
C18—C17—C16	120.7 (3)	C58—C57—C56	120.7 (3)
C18—C17—H17	119.6	C58—C57—H57	119.6
C16—C17—H17	119.6	C56—C57—H57	119.6
C17—C18—C19	120.5 (3)	C57—C58—C59	120.4 (3)
C17—C18—H18	119.7	C57—C58—H58	119.8
C19—C18—H18	119.7	C59—C58—H58	119.8
C20—C19—C18	119.0 (3)	C60—C59—C58	118.8 (3)
C20—C19—N3	116.3 (2)	C60—C59—N43	116.3 (2)
C18—C19—N3	124.7 (2)	C58—C59—N43	124.9 (3)
C19—C20—C15	121.4 (2)	C59—C60—C55	121.6 (3)
C19—C20—H20	119.3	C59—C60—H60	119.2
C15—C20—H20	119.3	C55—C60—H60	119.2
C22—C21—C26	119.2 (3)	C66—C61—C62	119.7 (3)
C22—C21—N4	125.4 (2)	C66—C61—N44	115.8 (3)
C26—C21—N4	115.4 (2)	C62—C61—N44	124.6 (3)
C21—C22—C23	120.2 (3)	C63—C62—C61	119.8 (3)
C21—C22—H22	119.9	C63—C62—H62	120.1
C23—C22—H22	119.9	C61—C62—H62	120.1
C22—C23—C24	121.4 (3)	C62—C63—C64	121.6 (3)
C22—C23—H23	119.3	C62—C63—H63	119.2
C24—C23—H23	119.3	C64—C63—H63	119.2
C25—C24—C23	117.9 (3)	C65—C64—C63	117.8 (3)
C25—C24—C28	121.7 (3)	C65—C64—C68	121.0 (3)
C23—C24—C28	120.4 (3)	C63—C64—C68	121.2 (3)
C24—C25—C26	121.2 (3)	C64—C65—C66	121.3 (3)
C24—C25—H25	119.4	C64—C65—H65	119.3
C26—C25—H25	119.4	C66—C65—H65	119.3
C21—C26—C25	120.1 (3)	C61—C66—C65	119.8 (3)
C21—C26—H26	119.9	C61—C66—H66	120.1
C25—C26—H26	119.9	C65—C66—H66	120.1
C11—C27—H271	109.5	C51—C67—H671	109.5
C11—C27—H272	109.5	C51—C67—H672	109.5
H271—C27—H272	109.5	H671—C67—H672	109.5
C11—C27—H273	109.5	C51—C67—H673	109.5
H271—C27—H273	109.5	H671—C67—H673	109.5
H272—C27—H273	109.5	H672—C67—H673	109.5
C24—C28—H281	109.5	C64—C68—H681	109.5
C24—C28—H282	109.5	C64—C68—H682	109.5
H281—C28—H282	109.5	H681—C68—H682	109.5
C24—C28—H283	109.5	C64—C68—H683	109.5
H281—C28—H283	109.5	H681—C68—H683	109.5
H282—C28—H283	109.5	H682—C68—H683	109.5

Sn1—C29—H291	109.5	Sn2—C69—H691	109.5
Sn1—C29—H292	109.5	Sn2—C69—H692	109.5
H291—C29—H292	109.5	H691—C69—H692	109.5
Sn1—C29—H293	109.5	Sn2—C69—H693	109.5
H291—C29—H293	109.5	H691—C69—H693	109.5
H292—C29—H293	109.5	H692—C69—H693	109.5
Sn1—C30—H301	109.5	Sn2—C70—H701	109.5
Sn1—C30—H302	109.5	Sn2—C70—H702	109.5
H301—C30—H302	109.5	H701—C70—H702	109.5
Sn1—C30—H303	109.5	Sn2—C70—H703	109.5
H301—C30—H303	109.5	H701—C70—H703	109.5
H302—C30—H303	109.5	H702—C70—H703	109.5

C6—N1—N2—C8	179.6 (2)	C46—N41—N42—C48	179.2 (2)
C19—N3—N4—C21	178.0 (2)	C59—N43—N44—C61	177.4 (2)
Sn1—O2—C1—O1	2.1 (2)	Sn2—O42—C41—O41	−5.3 (2)
Sn1—O2—C1—C2	−176.6 (3)	Sn2—O42—C41—C42	172.6 (3)
Sn1—O1—C1—O2	−2.7 (3)	Sn2—O41—C41—O42	6.6 (3)
Sn1—O1—C1—C2	176.1 (2)	Sn2—O41—C41—C42	−171.4 (2)
O2—C1—C2—C7	178.5 (3)	O42—C41—C42—C47	−174.7 (3)
O1—C1—C2—C7	−0.2 (4)	O41—C41—C42—C47	3.1 (4)
O2—C1—C2—C3	0.1 (4)	O42—C41—C42—C43	3.7 (4)
O1—C1—C2—C3	−178.6 (3)	O41—C41—C42—C43	−178.4 (2)
C7—C2—C3—O3	−178.6 (3)	C47—C42—C43—O43	−179.2 (3)
C1—C2—C3—O3	−0.3 (4)	C41—C42—C43—O43	2.3 (4)
C7—C2—C3—C4	−0.5 (4)	C47—C42—C43—C44	0.5 (4)
C1—C2—C3—C4	177.9 (3)	C41—C42—C43—C44	−177.9 (3)
O3—C3—C4—C5	179.3 (3)	O43—C43—C44—C45	179.1 (3)
C2—C3—C4—C5	1.0 (4)	C42—C43—C44—C45	−0.7 (4)
C3—C4—C5—C6	−0.4 (4)	C43—C44—C45—C46	0.6 (4)
C4—C5—C6—C7	−0.7 (4)	C44—C45—C46—C47	−0.3 (4)
C4—C5—C6—N1	−179.6 (3)	C44—C45—C46—N41	179.5 (3)
N2—N1—C6—C7	173.6 (2)	N42—N41—C46—C47	172.7 (2)
N2—N1—C6—C5	−7.5 (4)	N42—N41—C46—C45	−7.2 (4)
C5—C6—C7—C2	1.3 (4)	C45—C46—C47—C42	0.2 (4)
N1—C6—C7—C2	−179.7 (3)	N41—C46—C47—C42	−179.7 (2)
C3—C2—C7—C6	−0.7 (4)	C43—C42—C47—C46	−0.3 (4)
C1—C2—C7—C6	−179.0 (3)	C41—C42—C47—C46	178.2 (3)
N1—N2—C8—C13	176.6 (3)	N41—N42—C48—C53	−175.5 (2)
N1—N2—C8—C9	−4.6 (4)	N41—N42—C48—C49	5.3 (4)
C13—C8—C9—C10	−2.4 (5)	C53—C48—C49—C50	1.8 (4)
N2—C8—C9—C10	178.8 (3)	N42—C48—C49—C50	−179.0 (3)
C8—C9—C10—C11	0.9 (5)	C48—C49—C50—C51	−0.1 (5)
C9—C10—C11—C12	0.9 (5)	C49—C50—C51—C52	−0.6 (5)
C9—C10—C11—C27	−179.3 (3)	C49—C50—C51—C67	178.1 (3)
C10—C11—C12—C13	−1.2 (5)	C50—C51—C52—C53	−0.5 (4)
C27—C11—C12—C13	179.0 (3)	C67—C51—C52—C53	−179.2 (3)
C9—C8—C13—C12	2.1 (5)	C51—C52—C53—C48	2.3 (4)

N2—C8—C13—C12	−179.0 (3)	C49—C48—C53—C52	−2.9 (4)
C11—C12—C13—C8	−0.3 (5)	N42—C48—C53—C52	177.8 (3)
Sn1—O5—C14—O4	−2.5 (2)	Sn2—O45—C54—O44	−0.8 (2)
Sn1—O5—C14—C15	176.8 (3)	Sn2—O45—C54—C55	178.9 (3)
Sn1—O4—C14—O5	3.3 (3)	Sn2—O44—C54—O45	1.1 (3)
Sn1—O4—C14—C15	−176.1 (2)	Sn2—O44—C54—C55	−178.6 (2)
O5—C14—C15—C20	−175.0 (3)	O45—C54—C55—C60	175.8 (3)
O4—C14—C15—C20	4.4 (4)	O44—C54—C55—C60	−4.5 (4)
O5—C14—C15—C16	5.8 (4)	O45—C54—C55—C56	−5.5 (4)
O4—C14—C15—C16	−174.8 (3)	O44—C54—C55—C56	174.2 (2)
C20—C15—C16—O6	−178.3 (3)	C60—C55—C56—O46	−178.9 (3)
C14—C15—C16—O6	1.0 (4)	C54—C55—C56—O46	2.5 (4)
C20—C15—C16—C17	1.1 (4)	C60—C55—C56—C57	2.6 (4)
C14—C15—C16—C17	−179.6 (3)	C54—C55—C56—C57	−176.1 (3)
O6—C16—C17—C18	178.7 (3)	O46—C56—C57—C58	178.8 (3)
C15—C16—C17—C18	−0.7 (4)	C55—C56—C57—C58	−2.6 (4)
C16—C17—C18—C19	0.5 (4)	C56—C57—C58—C59	0.5 (4)
C17—C18—C19—C20	−0.9 (4)	C57—C58—C59—C60	1.7 (4)
C17—C18—C19—N3	−178.4 (3)	C57—C58—C59—N43	−177.7 (3)
N4—N3—C19—C20	168.4 (3)	N44—N43—C59—C60	175.9 (2)
N4—N3—C19—C18	−14.0 (4)	N44—N43—C59—C58	−4.6 (4)
C18—C19—C20—C15	1.4 (4)	C58—C59—C60—C55	−1.7 (4)
N3—C19—C20—C15	179.1 (2)	N43—C59—C60—C55	177.7 (2)
C16—C15—C20—C19	−1.5 (4)	C56—C55—C60—C59	−0.4 (4)
C14—C15—C20—C19	179.2 (3)	C54—C55—C60—C59	178.3 (3)
N3—N4—C21—C22	−9.6 (4)	N43—N44—C61—C66	166.8 (3)
N3—N4—C21—C26	172.1 (3)	N43—N44—C61—C62	−14.1 (4)
C26—C21—C22—C23	0.1 (5)	C66—C61—C62—C63	−1.2 (4)
N4—C21—C22—C23	−178.2 (3)	N44—C61—C62—C63	179.7 (3)
C21—C22—C23—C24	0.1 (5)	C61—C62—C63—C64	−0.1 (5)
C22—C23—C24—C25	0.1 (5)	C62—C63—C64—C65	1.7 (5)
C22—C23—C24—C28	−180.0 (3)	C62—C63—C64—C68	−178.3 (3)
C23—C24—C25—C26	−0.3 (5)	C63—C64—C65—C66	−1.9 (5)
C28—C24—C25—C26	179.7 (3)	C68—C64—C65—C66	178.1 (3)
C22—C21—C26—C25	−0.4 (5)	C62—C61—C66—C65	1.0 (5)
N4—C21—C26—C25	178.1 (3)	N44—C61—C66—C65	−179.9 (3)
C24—C25—C26—C21	0.5 (5)	C64—C65—C66—C61	0.6 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O2	0.80 (4)	1.89 (4)	2.611 (3)	150 (4)
O6—H6···O5	0.75 (3)	2.00 (3)	2.634 (3)	142 (4)
O6—H6···O42	0.75 (3)	2.35 (3)	2.887 (3)	130 (3)
O43—H43···O5	0.72 (3)	2.62 (3)	3.151 (3)	132 (3)
O43—H43···O42	0.72 (3)	2.01 (3)	2.642 (3)	146 (4)
O46—H46···O45	0.84 (3)	1.89 (3)	2.618 (3)	145 (3)
C29—H292···O43	0.98	2.37	3.314 (4)	162

C30—H303···O46^{i}	0.98	2.58	3.357 (4)	136
C68—H681···O44^{ii}	0.98	2.56	3.463 (4)	153
C69—H691···O2^{iii}	0.98	2.55	3.443 (4)	151
C12—H12···*Cg*7^{iv}	0.95	3.00	3.833 (3)	147
C68—H683···*Cg*5^{v}	0.98	2.86	3.625 (3)	136

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) −*x*−2, −*y*−1, −*z*; (iii) *x*−1, *y*, *z*; (iv) −*x*, −*y*+1, −*z*+1; (v) *x*−1, *y*−1, *z*.

(II) Di-*n*-butylbis{2-hydroxy-5-[(*E*)-2-(4-methylphenyl)diazen-1-yl]benzoato}tin(IV) benzene hemisolvate

Crystal data

$[Sn(C_4H_9)_2(C_{14}H_{11}N_2O_3)_2]\cdot 0.5C_6H_6$
M_r = 1564.92
Triclinic, $P\overline{1}$
a = 12.0462 (1) Å
b = 13.6264 (2) Å
c = 22.8143 (3) Å
α = 102.2665 (6)°
β = 100.3180 (6)°
γ = 91.6029 (6)°
V = 3591.71 (8) Å^3
Z = 2
F(000) = 1612
D_x = 1.447 Mg m^{-3}
Melting point: 448 K
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 87809 reflections
θ = 2.0–27.5°
μ = 0.76 mm^{-1}
T = 160 K
Prism, orange
0.23 × 0.18 × 0.18 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: Nonius FR590 sealed tube generator
Horizontally mounted graphite crystal monochromator
Detector resolution: 9 pixels mm^{-1}
φ and *ω* scans with *κ* offsets
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.802, T_{max} = 0.881
76914 measured reflections
16442 independent reflections
10227 reflections with $I > 2\sigma(I)$
R_{int} = 0.083
θ_{max} = 27.5°, θ_{min} = 2.1°
h = −15→15
k = −17→17
l = −29→29

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.117
S = 1.03
16442 reflections
971 parameters
181 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0557P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 1.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.95 e Å^{-3}

Special details

Experimental. Solvent used: benzene Cooling Device: Oxford Cryosystems Cryostream 700 Crystal mount: glued on a glass fibre Mosaicity (°.): 0.725 (1) Frames collected: 540 Seconds exposure per frame: 14 Degrees rotation per frame: 1.4 Crystal-Detector distance (mm): 34.0

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. In each independent molecule of the Sn complex in the structure of (II), the outer three C-atoms of one *n*-butyl group are disordered over two conformations. Refinement of the site occupation factors for the two orientations yielded values of 0.718 (6) and 0.541 (5) for the major conformation of molecules A (containing atom Sn1) and B (containing atom Sn2), respectively. Similarity restraints were applied to the chemically equivalent bond lengths and angles of all C-atoms in the *n*-butyl groups, including those of the ordered group in molecule A. In this way, the well defined geometry of the ordered *n*-butyl group helped to maintain reasonable geometry within the two conformations of the disordered ligands. The length of the first *n*-butyl C—C bond out from the Sn atom was also restrained to 1.520 (5) Å. Neighbouring C atoms within and between each conformation of the disordered *n*-butyl groups were restrained to have similar atomic displacement parameters.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Sn1	0.44920 (2)	0.59909 (2)	0.09762 (2)	0.03200 (8)	
O1	0.33833 (19)	0.50947 (16)	0.02250 (10)	0.0353 (6)	
O2	0.2592 (2)	0.65266 (16)	0.04583 (11)	0.0388 (6)	
O3	0.0608 (2)	0.67716 (17)	−0.01607 (12)	0.0443 (6)	
H3	0.1191	0.6934	0.0112	0.066*	
O4	0.5435 (2)	0.47234 (16)	0.08918 (11)	0.0366 (6)	
O5	0.6404 (2)	0.58034 (17)	0.16900 (11)	0.0407 (6)	
O6	0.8167 (2)	0.52092 (17)	0.23536 (12)	0.0449 (6)	
H6	0.7713	0.5622	0.2244	0.067*	
N1	0.0642 (2)	0.2813 (2)	−0.14326 (13)	0.0339 (7)	
N2	−0.0197 (2)	0.2482 (2)	−0.18465 (13)	0.0341 (7)	
N3	0.7190 (3)	0.1484 (2)	0.07225 (14)	0.0388 (7)	
N4	0.7796 (3)	0.0789 (2)	0.08239 (14)	0.0422 (8)	
C1	0.2547 (3)	0.5647 (2)	0.01351 (15)	0.0331 (8)	
C2	0.1560 (3)	0.5229 (2)	−0.03385 (15)	0.0280 (8)	
C3	0.0640 (3)	0.5815 (2)	−0.04607 (16)	0.0342 (8)	
C4	−0.0290 (3)	0.5392 (3)	−0.09142 (17)	0.0407 (9)	
H4	−0.0911	0.5787	−0.1001	0.049*	
C5	−0.0321 (3)	0.4414 (3)	−0.12360 (16)	0.0358 (8)	
H5	−0.0965	0.4135	−0.1539	0.043*	
C6	0.0595 (3)	0.3827 (2)	−0.11182 (15)	0.0304 (8)	
C7	0.1516 (3)	0.4234 (2)	−0.06746 (15)	0.0294 (8)	
H7	0.2135	0.3835	−0.0594	0.035*	
C8	−0.0168 (3)	0.1460 (2)	−0.21532 (15)	0.0316 (8)	
C9	0.0705 (3)	0.0847 (3)	−0.20264 (16)	0.0389 (9)	
H9	0.1349	0.1106	−0.1719	0.047*	
C10	0.0632 (3)	−0.0138 (3)	−0.23479 (17)	0.0420 (9)	
H10	0.1233	−0.0553	−0.2260	0.050*	
C11	−0.0298 (3)	−0.0535 (3)	−0.27958 (17)	0.0405 (9)	
C12	−0.1157 (3)	0.0084 (3)	−0.29292 (17)	0.0455 (10)	
H12	−0.1795	−0.0172	−0.3241	0.055*	
C13	−0.1088 (3)	0.1083 (3)	−0.26073 (16)	0.0408 (9)	
H13	−0.1678	0.1504	−0.2702	0.049*	
C14	0.6276 (3)	0.4939 (2)	0.13494 (16)	0.0320 (8)	
C15	0.7035 (3)	0.4144 (2)	0.14517 (15)	0.0307 (8)	
C16	0.7921 (3)	0.4304 (2)	0.19580 (16)	0.0332 (8)	

C17	0.8572 (3)	0.3515 (3)	0.20698 (17)	0.0397 (9)	
H17	0.9159	0.3619	0.2420	0.048*	
C18	0.8375 (3)	0.2579 (3)	0.16750 (17)	0.0401 (9)	
H18	0.8833	0.2047	0.1751	0.048*	
C19	0.7500 (3)	0.2417 (2)	0.11650 (16)	0.0330 (8)	
C20	0.6835 (3)	0.3192 (2)	0.10639 (16)	0.0330 (8)	
H20	0.6227	0.3075	0.0723	0.040*	
C21	0.7465 (3)	−0.0141 (3)	0.03794 (16)	0.0359 (9)	
C22	0.6494 (3)	−0.0296 (3)	−0.00670 (18)	0.0455 (10)	
H22	0.6004	0.0232	−0.0100	0.055*	
C23	0.6240 (3)	−0.1234 (3)	−0.04675 (17)	0.0438 (9)	
H23	0.5571	−0.1344	−0.0772	0.053*	
C24	0.6955 (3)	−0.2008 (3)	−0.04261 (17)	0.0377 (9)	
C25	0.7919 (3)	−0.1834 (3)	0.00258 (17)	0.0447 (10)	
H25	0.8416	−0.2357	0.0059	0.054*	
C26	0.8166 (3)	−0.0916 (3)	0.04264 (17)	0.0448 (10)	
H26	0.8824	−0.0814	0.0738	0.054*	
C27	−0.0388 (4)	−0.1633 (3)	−0.31433 (19)	0.0546 (12)	
H271	0.0365	−0.1894	−0.3104	0.082*	
H272	−0.0702	−0.1677	−0.3576	0.082*	
H273	−0.0885	−0.2033	−0.2973	0.082*	
C28	0.6685 (3)	−0.3021 (3)	−0.08653 (18)	0.0496 (11)	
H281	0.5883	−0.3226	−0.0911	0.074*	
H282	0.7148	−0.3521	−0.0706	0.074*	
H283	0.6851	−0.2972	−0.1264	0.074*	
C29	0.3650 (3)	0.5830 (3)	0.16937 (17)	0.0433 (10)	
H291	0.2900	0.5475	0.1509	0.052*	
H292	0.4085	0.5390	0.1931	0.052*	
C30	0.3475 (4)	0.6780 (3)	0.21331 (18)	0.0596 (12)	
H301	0.2900	0.6638	0.2370	0.072*	
H302	0.3190	0.7289	0.1902	0.072*	
C31	0.4590 (4)	0.7200 (4)	0.2574 (2)	0.0743 (15)	
H311	0.4858	0.6697	0.2813	0.089*	
H312	0.5171	0.7314	0.2334	0.089*	
C32	0.4460 (4)	0.8152 (4)	0.2996 (2)	0.0817 (16)	
H321	0.4185	0.8650	0.2762	0.123*	
H322	0.5192	0.8403	0.3259	0.123*	
H323	0.3915	0.8035	0.3250	0.123*	
C33	0.5362 (3)	0.7035 (2)	0.06225 (16)	0.0410 (9)	
H331	0.5954	0.6681	0.0427	0.049*	0.718 (6)
H332	0.4820	0.7239	0.0297	0.049*	0.718 (6)
H333	0.6174	0.7067	0.0810	0.049*	0.282 (6)
H334	0.5298	0.6762	0.0179	0.049*	0.282 (6)
C34A	0.5916 (5)	0.7974 (3)	0.1063 (2)	0.0485 (15)	0.718 (6)
H341	0.6410	0.8321	0.0856	0.058*	0.718 (6)
H342	0.6405	0.7778	0.1411	0.058*	0.718 (6)
C35A	0.5106 (6)	0.8710 (7)	0.1310 (4)	0.067 (2)	0.718 (6)
H351	0.4603	0.8899	0.0964	0.081*	0.718 (6)

H352	0.4628	0.8377	0.1532	0.081*	0.718 (6)
C36A	0.5708 (7)	0.9646 (5)	0.1734 (3)	0.079 (2)	0.718 (6)
H361	0.5153	1.0076	0.1905	0.118*	0.718 (6)
H362	0.6127	1.0012	0.1506	0.118*	0.718 (6)
H363	0.6236	0.9461	0.2066	0.118*	0.718 (6)
C34B	0.4994 (11)	0.8094 (5)	0.0710 (6)	0.044 (2)	0.282 (6)
H343	0.4259	0.8088	0.0433	0.053*	0.282 (6)
H344	0.5550	0.8513	0.0582	0.053*	0.282 (6)
C35B	0.4865 (14)	0.860 (2)	0.1356 (8)	0.061 (4)	0.282 (6)
H353	0.4361	0.9160	0.1338	0.073*	0.282 (6)
H354	0.4512	0.8109	0.1541	0.073*	0.282 (6)
C36B	0.5992 (16)	0.9004 (17)	0.1745 (7)	0.089 (5)	0.282 (6)
H364	0.6416	0.9367	0.1519	0.134*	0.282 (6)
H365	0.6418	0.8444	0.1851	0.134*	0.282 (6)
H366	0.5877	0.9463	0.2120	0.134*	0.282 (6)
Sn2	0.59619 (2)	0.66771 (2)	0.49220 (2)	0.02954 (8)	
O41	0.6835 (2)	0.53667 (16)	0.48649 (11)	0.0362 (6)	
O42	0.79209 (19)	0.64877 (15)	0.55971 (10)	0.0342 (5)	
O43	0.9810 (2)	0.59333 (17)	0.61777 (11)	0.0403 (6)	
H43	0.9320	0.6335	0.6094	0.061*	
O44	0.48199 (19)	0.57754 (16)	0.41943 (11)	0.0387 (6)	
O45	0.40301 (19)	0.72170 (16)	0.43866 (10)	0.0346 (6)	
O46	0.2034 (2)	0.74147 (16)	0.37532 (11)	0.0370 (6)	
H46	0.2549	0.7557	0.4065	0.056*	
N41	0.8703 (2)	0.2176 (2)	0.46087 (13)	0.0333 (7)	
N42	0.9407 (2)	0.1516 (2)	0.46245 (13)	0.0339 (7)	
N43	0.2245 (3)	0.3468 (2)	0.24958 (13)	0.0376 (7)	
N44	0.1498 (2)	0.3132 (2)	0.20366 (13)	0.0336 (7)	
C41	0.7749 (3)	0.5608 (2)	0.52757 (15)	0.0288 (8)	
C42	0.8542 (3)	0.4826 (2)	0.53486 (15)	0.0272 (7)	
C43	0.9531 (3)	0.5030 (2)	0.57958 (16)	0.0310 (8)	
C44	1.0267 (3)	0.4255 (2)	0.58553 (17)	0.0372 (9)	
H44	1.0934	0.4380	0.6161	0.045*	
C45	1.0024 (3)	0.3323 (3)	0.54739 (16)	0.0345 (8)	
H45	1.0530	0.2809	0.5516	0.041*	
C46	0.9052 (3)	0.3117 (2)	0.50278 (15)	0.0296 (8)	
C47	0.8311 (3)	0.3864 (2)	0.49697 (15)	0.0279 (7)	
H47	0.7638	0.3722	0.4669	0.033*	
C48	0.9028 (3)	0.0582 (2)	0.42035 (16)	0.0322 (8)	
C49	0.7972 (3)	0.0381 (3)	0.38221 (17)	0.0373 (9)	
H49	0.7443	0.0886	0.3827	0.045*	
C50	0.7699 (3)	−0.0548 (3)	0.34394 (17)	0.0396 (9)	
H50	0.6976	−0.0680	0.3181	0.048*	
C51	0.8457 (3)	−0.1309 (3)	0.34199 (17)	0.0394 (9)	
C52	0.9500 (3)	−0.1095 (2)	0.37948 (17)	0.0382 (9)	
H52	1.0031	−0.1598	0.3784	0.046*	
C53	0.9797 (3)	−0.0162 (2)	0.41902 (16)	0.0353 (8)	
H53	1.0520	−0.0032	0.4449	0.042*	

C54	0.3990 (3)	0.6328 (2)	0.40817 (15)	0.0298 (8)	
C55	0.3032 (3)	0.5893 (2)	0.35965 (15)	0.0283 (7)	
C56	0.2098 (3)	0.6457 (2)	0.34531 (15)	0.0282 (8)	
C57	0.1204 (3)	0.6022 (2)	0.29813 (15)	0.0322 (8)	
H57	0.0573	0.6402	0.2887	0.039*	
C58	0.1218 (3)	0.5055 (2)	0.26506 (15)	0.0320 (8)	
H58	0.0607	0.4773	0.2327	0.038*	
C59	0.2141 (3)	0.4491 (2)	0.27952 (15)	0.0305 (8)	
C60	0.3028 (3)	0.4905 (2)	0.32604 (15)	0.0327 (8)	
H60	0.3648	0.4514	0.3355	0.039*	
C61	0.1580 (3)	0.2091 (2)	0.17527 (15)	0.0323 (8)	
C62	0.2366 (3)	0.1480 (3)	0.19879 (17)	0.0424 (9)	
H62	0.2908	0.1742	0.2349	0.051*	
C63	0.2345 (3)	0.0484 (3)	0.16858 (17)	0.0458 (10)	
H63	0.2873	0.0062	0.1850	0.055*	
C64	0.1587 (3)	0.0082 (3)	0.11554 (17)	0.0412 (10)	
C65	0.0818 (3)	0.0715 (3)	0.09272 (17)	0.0421 (9)	
H65	0.0284	0.0456	0.0562	0.051*	
C66	0.0816 (3)	0.1710 (3)	0.12207 (16)	0.0392 (9)	
H66	0.0288	0.2131	0.1056	0.047*	
C67	0.8131 (3)	−0.2332 (3)	0.29954 (17)	0.0456 (10)	
H671	0.7388	−0.2580	0.3043	0.068*	
H672	0.8695	−0.2804	0.3097	0.068*	
H673	0.8099	−0.2273	0.2572	0.068*	
C68	0.1583 (4)	−0.1011 (3)	0.08387 (18)	0.0505 (11)	
H681	0.0941	−0.1178	0.0495	0.076*	
H682	0.1515	−0.1437	0.1129	0.076*	
H683	0.2290	−0.1128	0.0687	0.076*	
C69	0.6876 (3)	0.7558 (2)	0.44813 (16)	0.0354 (8)	
H691	0.7516	0.7179	0.4357	0.042*	
H692	0.6374	0.7645	0.4105	0.042*	
C70	0.7342 (3)	0.8596 (2)	0.48601 (17)	0.0377 (9)	
H701	0.7735	0.8529	0.5268	0.045*	
H702	0.7905	0.8872	0.4660	0.045*	
C71	0.6423 (3)	0.9328 (3)	0.49370 (18)	0.0428 (10)	
H711	0.6045	0.9410	0.4529	0.051*	
H712	0.5849	0.9043	0.5126	0.051*	
C72	0.6880 (3)	1.0353 (3)	0.53290 (19)	0.0496 (11)	
H721	0.7248	1.0277	0.5735	0.074*	
H722	0.6255	1.0793	0.5368	0.074*	
H723	0.7431	1.0649	0.5137	0.074*	
C73	0.5172 (3)	0.6722 (3)	0.56841 (16)	0.0406 (9)	
H731	0.4405	0.6957	0.5587	0.049*	0.459 (5)
H732	0.5084	0.6027	0.5744	0.049*	0.459 (5)
H733	0.4488	0.6251	0.5556	0.049*	0.541 (5)
H734	0.5695	0.6478	0.6001	0.049*	0.541 (5)
C74A	0.5793 (6)	0.7393 (4)	0.6286 (3)	0.0426 (18)	0.459 (5)
H741	0.5328	0.7367	0.6600	0.051*	0.459 (5)

H742	0.6510	0.7090	0.6410	0.051*	0.459 (5)
C75A	0.6075 (8)	0.8498 (6)	0.6303 (10)	0.045 (3)	0.459 (5)
H751	0.6551	0.8815	0.6703	0.055*	0.459 (5)
H752	0.6516	0.8544	0.5982	0.055*	0.459 (5)
C76A	0.5026 (8)	0.9061 (6)	0.6205 (5)	0.056 (3)	0.459 (5)
H761	0.4583	0.9010	0.6520	0.084*	0.459 (5)
H762	0.4572	0.8770	0.5801	0.084*	0.459 (5)
H763	0.5241	0.9771	0.6232	0.084*	0.459 (5)
C74B	0.4838 (5)	0.7743 (4)	0.5961 (3)	0.0401 (17)	0.541 (5)
H743	0.4273	0.7679	0.6219	0.048*	0.541 (5)
H744	0.4499	0.8081	0.5635	0.048*	0.541 (5)
C75B	0.5896 (7)	0.8355 (6)	0.6347 (8)	0.047 (2)	0.541 (5)
H753	0.6260	0.7988	0.6653	0.056*	0.541 (5)
H754	0.6440	0.8446	0.6082	0.056*	0.541 (5)
C76B	0.5598 (7)	0.9374 (5)	0.6671 (4)	0.064 (2)	0.541 (5)
H764	0.6283	0.9748	0.6928	0.097*	0.541 (5)
H765	0.5047	0.9283	0.6926	0.097*	0.541 (5)
H766	0.5271	0.9750	0.6367	0.097*	0.541 (5)
C80	0.5366 (4)	0.3454 (4)	0.2498 (2)	0.0760 (14)	
H80	0.4710	0.3621	0.2249	0.091*	
C81	0.5734 (4)	0.2499 (4)	0.2372 (2)	0.0677 (14)	
H81	0.5328	0.2010	0.2036	0.081*	
C82	0.6672 (4)	0.2246 (4)	0.2721 (2)	0.0676 (13)	
H82	0.6925	0.1586	0.2634	0.081*	
C83	0.7251 (4)	0.2975 (4)	0.3207 (2)	0.0713 (14)	
H83	0.7918	0.2819	0.3452	0.086*	
C84	0.6871 (4)	0.3912 (4)	0.3336 (2)	0.0668 (13)	
H84	0.7262	0.4399	0.3678	0.080*	
C85	0.5940 (5)	0.4159 (4)	0.2980 (2)	0.0698 (14)	
H85	0.5690	0.4821	0.3067	0.084*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.03061 (15)	0.02481 (14)	0.03640 (16)	0.00053 (10)	0.00358 (12)	0.00003 (11)
O1	0.0303 (14)	0.0280 (13)	0.0403 (14)	0.0043 (11)	−0.0027 (11)	−0.0006 (11)
O2	0.0418 (15)	0.0269 (13)	0.0416 (15)	0.0031 (11)	0.0024 (12)	−0.0015 (11)
O3	0.0473 (17)	0.0305 (14)	0.0464 (17)	0.0129 (12)	−0.0012 (13)	−0.0033 (12)
O4	0.0371 (15)	0.0272 (13)	0.0403 (15)	0.0031 (11)	−0.0005 (12)	0.0027 (11)
O5	0.0386 (15)	0.0286 (13)	0.0499 (16)	0.0048 (11)	0.0071 (13)	−0.0019 (12)
O6	0.0409 (16)	0.0276 (14)	0.0533 (17)	−0.0008 (12)	−0.0076 (13)	−0.0051 (12)
N1	0.0354 (18)	0.0296 (16)	0.0348 (17)	−0.0001 (14)	0.0026 (15)	0.0063 (13)
N2	0.0372 (18)	0.0307 (16)	0.0321 (17)	0.0008 (14)	0.0042 (15)	0.0042 (13)
N3	0.044 (2)	0.0290 (16)	0.0454 (19)	0.0085 (15)	0.0142 (16)	0.0081 (14)
N4	0.043 (2)	0.0366 (18)	0.045 (2)	0.0013 (16)	0.0058 (16)	0.0085 (15)
C1	0.037 (2)	0.0274 (19)	0.035 (2)	0.0019 (16)	0.0097 (17)	0.0052 (16)
C2	0.0279 (19)	0.0259 (18)	0.0285 (19)	−0.0008 (15)	0.0052 (16)	0.0028 (14)
C3	0.043 (2)	0.0247 (18)	0.033 (2)	0.0093 (17)	0.0064 (18)	0.0025 (15)

C4	0.037 (2)	0.039 (2)	0.043 (2)	0.0139 (18)	0.0005 (19)	0.0065 (18)
C5	0.033 (2)	0.037 (2)	0.033 (2)	0.0042 (17)	−0.0008 (17)	0.0041 (16)
C6	0.033 (2)	0.0244 (18)	0.0319 (19)	0.0032 (15)	0.0048 (17)	0.0036 (15)
C7	0.0285 (19)	0.0269 (18)	0.0312 (19)	0.0054 (15)	0.0036 (16)	0.0045 (15)
C8	0.033 (2)	0.0302 (19)	0.030 (2)	−0.0004 (16)	0.0042 (16)	0.0047 (16)
C9	0.042 (2)	0.035 (2)	0.035 (2)	0.0017 (18)	−0.0002 (18)	0.0052 (17)
C10	0.052 (3)	0.031 (2)	0.041 (2)	0.0031 (18)	0.004 (2)	0.0064 (17)
C11	0.056 (3)	0.030 (2)	0.038 (2)	−0.0021 (19)	0.017 (2)	0.0059 (17)
C12	0.046 (3)	0.042 (2)	0.039 (2)	−0.0103 (19)	−0.0011 (19)	−0.0017 (18)
C13	0.035 (2)	0.039 (2)	0.042 (2)	0.0038 (17)	0.0008 (18)	0.0018 (18)
C14	0.029 (2)	0.031 (2)	0.036 (2)	−0.0006 (16)	0.0081 (17)	0.0053 (16)
C15	0.031 (2)	0.0259 (18)	0.036 (2)	0.0026 (15)	0.0115 (17)	0.0040 (15)
C16	0.030 (2)	0.0288 (19)	0.038 (2)	−0.0023 (16)	0.0062 (17)	0.0005 (16)
C17	0.029 (2)	0.038 (2)	0.048 (2)	−0.0002 (17)	−0.0009 (18)	0.0087 (18)
C18	0.035 (2)	0.033 (2)	0.055 (3)	0.0099 (17)	0.012 (2)	0.0128 (18)
C19	0.039 (2)	0.0269 (19)	0.036 (2)	0.0013 (16)	0.0150 (18)	0.0055 (16)
C20	0.035 (2)	0.032 (2)	0.031 (2)	0.0037 (16)	0.0076 (17)	0.0039 (16)
C21	0.043 (2)	0.032 (2)	0.031 (2)	−0.0079 (17)	0.0097 (18)	−0.0001 (16)
C22	0.044 (2)	0.033 (2)	0.059 (3)	0.0062 (18)	0.013 (2)	0.0063 (19)
C23	0.040 (2)	0.037 (2)	0.047 (2)	−0.0037 (18)	0.0026 (19)	0.0002 (18)
C24	0.043 (2)	0.030 (2)	0.041 (2)	−0.0040 (17)	0.016 (2)	0.0051 (17)
C25	0.055 (3)	0.033 (2)	0.049 (2)	0.0076 (19)	0.015 (2)	0.0089 (18)
C26	0.053 (3)	0.038 (2)	0.044 (2)	0.0054 (19)	0.010 (2)	0.0069 (18)
C27	0.079 (3)	0.032 (2)	0.049 (3)	−0.005 (2)	0.019 (2)	−0.0039 (18)
C28	0.059 (3)	0.030 (2)	0.060 (3)	−0.0074 (19)	0.025 (2)	0.0007 (19)
C29	0.039 (2)	0.049 (2)	0.044 (2)	−0.0017 (18)	0.0126 (19)	0.0105 (19)
C30	0.058 (3)	0.066 (3)	0.052 (3)	−0.010 (2)	0.021 (2)	0.001 (2)
C31	0.060 (3)	0.092 (4)	0.066 (3)	−0.011 (3)	0.018 (3)	0.002 (3)
C32	0.079 (4)	0.082 (4)	0.072 (4)	−0.016 (3)	0.016 (3)	−0.007 (3)
C33	0.046 (2)	0.033 (2)	0.044 (2)	0.0010 (17)	0.0121 (19)	0.0051 (17)
C34A	0.054 (3)	0.037 (3)	0.056 (3)	−0.004 (2)	0.019 (3)	0.006 (2)
C35A	0.079 (4)	0.042 (4)	0.082 (4)	−0.015 (3)	0.036 (3)	0.003 (3)
C36A	0.104 (6)	0.041 (4)	0.083 (5)	−0.009 (4)	0.026 (4)	−0.010 (4)
C34B	0.057 (5)	0.028 (4)	0.055 (5)	0.002 (4)	0.030 (4)	0.007 (4)
C35B	0.081 (6)	0.034 (6)	0.073 (6)	−0.013 (6)	0.034 (6)	0.009 (5)
C36B	0.087 (10)	0.099 (10)	0.083 (9)	−0.011 (10)	0.020 (8)	0.020 (9)
Sn2	0.02860 (14)	0.01906 (13)	0.03559 (15)	0.00263 (10)	−0.00071 (11)	−0.00019 (10)
O41	0.0338 (14)	0.0254 (12)	0.0410 (15)	0.0060 (11)	−0.0068 (12)	−0.0001 (11)
O42	0.0343 (14)	0.0219 (12)	0.0403 (14)	0.0042 (10)	0.0002 (11)	−0.0010 (11)
O43	0.0337 (15)	0.0281 (13)	0.0485 (16)	0.0023 (11)	−0.0094 (12)	−0.0006 (12)
O44	0.0325 (14)	0.0234 (12)	0.0479 (15)	0.0049 (11)	−0.0122 (12)	−0.0028 (11)
O45	0.0346 (14)	0.0256 (13)	0.0384 (14)	0.0026 (11)	0.0009 (11)	0.0006 (11)
O46	0.0342 (15)	0.0280 (13)	0.0426 (16)	0.0082 (11)	−0.0020 (12)	0.0006 (11)
N41	0.0298 (17)	0.0266 (16)	0.0438 (19)	0.0067 (13)	0.0069 (14)	0.0076 (14)
N42	0.0319 (17)	0.0232 (15)	0.0467 (19)	0.0049 (13)	0.0097 (15)	0.0056 (13)
N43	0.0372 (19)	0.0322 (17)	0.0360 (18)	−0.0025 (14)	−0.0025 (15)	−0.0002 (14)
N44	0.0379 (18)	0.0282 (16)	0.0304 (17)	−0.0010 (13)	0.0030 (14)	−0.0002 (13)
C41	0.030 (2)	0.0239 (18)	0.031 (2)	0.0041 (15)	0.0042 (16)	0.0040 (15)

C42	0.0253 (19)	0.0244 (17)	0.0302 (19)	0.0028 (14)	0.0052 (16)	0.0027 (14)
C43	0.030 (2)	0.0251 (18)	0.035 (2)	−0.0035 (15)	0.0026 (16)	0.0038 (15)
C44	0.029 (2)	0.029 (2)	0.049 (2)	0.0002 (16)	−0.0033 (17)	0.0075 (17)
C45	0.0238 (19)	0.0311 (19)	0.050 (2)	0.0064 (15)	0.0045 (17)	0.0131 (17)
C46	0.031 (2)	0.0243 (18)	0.035 (2)	0.0035 (15)	0.0083 (17)	0.0079 (15)
C47	0.0271 (19)	0.0239 (17)	0.0297 (19)	0.0045 (14)	0.0001 (15)	0.0034 (14)
C48	0.031 (2)	0.0243 (18)	0.043 (2)	0.0029 (15)	0.0126 (18)	0.0080 (16)
C49	0.034 (2)	0.030 (2)	0.048 (2)	0.0101 (16)	0.0073 (19)	0.0069 (17)
C50	0.039 (2)	0.031 (2)	0.046 (2)	0.0031 (17)	0.0030 (19)	0.0058 (17)
C51	0.050 (3)	0.028 (2)	0.043 (2)	0.0016 (18)	0.020 (2)	0.0042 (17)
C52	0.038 (2)	0.0266 (19)	0.053 (2)	0.0090 (17)	0.017 (2)	0.0053 (17)
C53	0.030 (2)	0.0298 (19)	0.046 (2)	0.0052 (16)	0.0108 (18)	0.0058 (17)
C54	0.030 (2)	0.0244 (18)	0.033 (2)	0.0009 (15)	0.0035 (16)	0.0037 (15)
C55	0.0294 (19)	0.0271 (18)	0.0270 (19)	0.0018 (15)	0.0021 (15)	0.0059 (14)
C56	0.0285 (19)	0.0251 (18)	0.0304 (19)	0.0013 (15)	0.0080 (16)	0.0028 (15)
C57	0.0252 (19)	0.034 (2)	0.035 (2)	0.0045 (15)	−0.0024 (16)	0.0086 (16)
C58	0.0259 (19)	0.037 (2)	0.0297 (19)	−0.0030 (16)	−0.0013 (16)	0.0061 (16)
C59	0.035 (2)	0.0251 (18)	0.0287 (19)	−0.0011 (16)	0.0021 (16)	0.0033 (15)
C60	0.034 (2)	0.0235 (18)	0.036 (2)	0.0025 (15)	0.0009 (17)	0.0016 (15)
C61	0.039 (2)	0.0294 (19)	0.0281 (19)	−0.0009 (16)	0.0081 (17)	0.0043 (15)
C62	0.049 (3)	0.039 (2)	0.033 (2)	−0.0007 (19)	0.0024 (19)	−0.0007 (17)
C63	0.058 (3)	0.032 (2)	0.046 (2)	0.0095 (19)	0.008 (2)	0.0071 (18)
C64	0.051 (3)	0.033 (2)	0.039 (2)	−0.0028 (19)	0.017 (2)	0.0006 (18)
C65	0.040 (2)	0.038 (2)	0.041 (2)	−0.0076 (18)	0.0074 (19)	−0.0054 (18)
C66	0.034 (2)	0.040 (2)	0.037 (2)	−0.0065 (17)	0.0013 (18)	0.0018 (17)
C67	0.052 (3)	0.033 (2)	0.047 (2)	0.0013 (19)	0.013 (2)	−0.0019 (18)
C68	0.066 (3)	0.030 (2)	0.050 (3)	−0.0072 (19)	0.018 (2)	−0.0085 (18)
C69	0.031 (2)	0.035 (2)	0.039 (2)	0.0041 (16)	0.0084 (17)	0.0058 (17)
C70	0.032 (2)	0.034 (2)	0.047 (2)	−0.0016 (16)	0.0093 (18)	0.0071 (17)
C71	0.040 (2)	0.032 (2)	0.056 (3)	0.0004 (17)	0.007 (2)	0.0120 (18)
C72	0.046 (3)	0.030 (2)	0.070 (3)	0.0027 (18)	0.012 (2)	0.005 (2)
C73	0.040 (2)	0.038 (2)	0.046 (2)	−0.0010 (17)	0.0124 (18)	0.0115 (17)
C74A	0.051 (4)	0.032 (3)	0.042 (4)	0.005 (3)	0.006 (3)	0.005 (3)
C75A	0.053 (5)	0.040 (4)	0.038 (5)	−0.003 (4)	0.004 (4)	0.002 (4)
C76A	0.054 (6)	0.048 (5)	0.066 (6)	0.016 (4)	0.007 (5)	0.018 (5)
C74B	0.037 (3)	0.040 (3)	0.042 (3)	0.001 (3)	0.013 (3)	0.002 (3)
C75B	0.052 (4)	0.051 (4)	0.033 (4)	0.004 (4)	0.007 (4)	−0.002 (4)
C76B	0.071 (6)	0.052 (5)	0.056 (5)	−0.003 (4)	0.006 (5)	−0.014 (4)
C80	0.063 (3)	0.089 (4)	0.068 (4)	0.007 (3)	0.000 (3)	0.009 (3)
C81	0.064 (3)	0.080 (4)	0.053 (3)	−0.017 (3)	0.015 (3)	0.000 (3)
C82	0.069 (4)	0.077 (3)	0.061 (3)	0.008 (3)	0.025 (3)	0.014 (3)
C83	0.050 (3)	0.100 (4)	0.062 (3)	0.003 (3)	0.003 (3)	0.022 (3)
C84	0.071 (4)	0.076 (4)	0.050 (3)	−0.020 (3)	0.012 (3)	0.008 (3)
C85	0.076 (4)	0.068 (3)	0.065 (3)	0.000 (3)	0.021 (3)	0.008 (3)

Geometric parameters (Å, º)

Sn1—O1	2.100 (2)	O41—C41	1.296 (4)
Sn1—O2	2.581 (2)	O42—C41	1.255 (4)
Sn1—O4	2.087 (2)	O43—C43	1.343 (4)
Sn1—O5	2.625 (3)	O43—H43	0.8400
Sn1—C29	2.119 (3)	O44—C54	1.291 (4)
Sn1—C33	2.117 (3)	O45—C54	1.257 (4)
O1—C1	1.287 (4)	O46—C56	1.350 (4)
O2—C1	1.261 (4)	O46—H46	0.8400
O3—C3	1.342 (4)	N41—N42	1.256 (4)
O3—H3	0.8400	N41—C46	1.428 (4)
O4—C14	1.295 (4)	N42—C48	1.429 (4)
O5—C14	1.255 (4)	N43—N44	1.246 (4)
O6—C16	1.354 (4)	N43—C59	1.436 (4)
O6—H6	0.8400	N44—C61	1.443 (4)
N1—N2	1.252 (4)	C41—C42	1.467 (4)
N1—C6	1.423 (4)	C42—C47	1.398 (4)
N2—C8	1.424 (4)	C42—C43	1.401 (5)
N3—N4	1.247 (4)	C43—C44	1.411 (5)
N3—C19	1.438 (4)	C44—C45	1.369 (5)
N4—C21	1.441 (4)	C44—H44	0.9500
C1—C2	1.465 (5)	C45—C46	1.385 (5)
C2—C7	1.402 (4)	C45—H45	0.9500
C2—C3	1.406 (5)	C46—C47	1.385 (4)
C3—C4	1.397 (5)	C47—H47	0.9500
C4—C5	1.375 (5)	C48—C49	1.390 (5)
C4—H4	0.9500	C48—C53	1.391 (4)
C5—C6	1.401 (5)	C49—C50	1.371 (5)
C5—H5	0.9500	C49—H49	0.9500
C6—C7	1.374 (5)	C50—C51	1.399 (5)
C7—H7	0.9500	C50—H50	0.9500
C8—C13	1.377 (5)	C51—C52	1.372 (5)
C8—C9	1.389 (5)	C51—C67	1.515 (5)
C9—C10	1.379 (5)	C52—C53	1.390 (5)
C9—H9	0.9500	C52—H52	0.9500
C10—C11	1.383 (5)	C53—H53	0.9500
C10—H10	0.9500	C54—C55	1.460 (5)
C11—C12	1.386 (5)	C55—C60	1.400 (4)
C11—C27	1.528 (5)	C55—C56	1.410 (5)
C12—C13	1.394 (5)	C56—C57	1.396 (5)
C12—H12	0.9500	C57—C58	1.374 (4)
C13—H13	0.9500	C57—H57	0.9500
C14—C15	1.466 (5)	C58—C59	1.400 (5)
C15—C20	1.393 (4)	C58—H58	0.9500
C15—C16	1.400 (5)	C59—C60	1.376 (5)
C16—C17	1.390 (5)	C60—H60	0.9500
C17—C18	1.382 (5)	C61—C66	1.376 (5)

C17—H17	0.9500	C61—C62	1.390 (5)
C18—C19	1.397 (5)	C62—C63	1.383 (5)
C18—H18	0.9500	C62—H62	0.9500
C19—C20	1.377 (5)	C63—C64	1.376 (5)
C20—H20	0.9500	C63—H63	0.9500
C21—C26	1.380 (5)	C64—C65	1.391 (5)
C21—C22	1.385 (5)	C64—C68	1.511 (5)
C22—C23	1.393 (5)	C65—C66	1.379 (5)
C22—H22	0.9500	C65—H65	0.9500
C23—C24	1.388 (5)	C66—H66	0.9500
C23—H23	0.9500	C67—H671	0.9800
C24—C25	1.386 (5)	C67—H672	0.9800
C24—C28	1.512 (5)	C67—H673	0.9800
C25—C26	1.373 (5)	C68—H681	0.9800
C25—H25	0.9500	C68—H682	0.9800
C26—H26	0.9500	C68—H683	0.9800
C27—H271	0.9800	C69—C70	1.525 (5)
C27—H272	0.9800	C69—H691	0.9900
C27—H273	0.9800	C69—H692	0.9900
C28—H281	0.9800	C70—C71	1.520 (5)
C28—H282	0.9800	C70—H701	0.9900
C28—H283	0.9800	C70—H702	0.9900
C29—C30	1.506 (5)	C71—C72	1.517 (5)
C29—H291	0.9900	C71—H711	0.9900
C29—H292	0.9900	C71—H712	0.9900
C30—C31	1.540 (5)	C72—H721	0.9800
C30—H301	0.9900	C72—H722	0.9800
C30—H302	0.9900	C72—H723	0.9800
C31—C32	1.473 (5)	C73—C74B	1.499 (5)
C31—H311	0.9900	C73—C74A	1.529 (5)
C31—H312	0.9900	C73—H731	0.9900
C32—H321	0.9800	C73—H732	0.9900
C32—H322	0.9800	C73—H733	0.9900
C32—H323	0.9800	C73—H734	0.9900
C33—C34A	1.503 (4)	C74A—C75A	1.525 (8)
C33—C34B	1.506 (5)	C74A—H741	0.9900
C33—H331	0.9900	C74A—H742	0.9900
C33—H332	0.9900	C75A—C76A	1.503 (8)
C33—H333	0.9900	C75A—H751	0.9900
C33—H334	0.9900	C75A—H752	0.9900
C34A—C35A	1.512 (7)	C76A—H761	0.9800
C34A—H341	0.9900	C76A—H762	0.9800
C34A—H342	0.9900	C76A—H763	0.9800
C35A—C36A	1.504 (7)	C74B—C75B	1.524 (8)
C35A—H351	0.9900	C74B—H743	0.9900
C35A—H352	0.9900	C74B—H744	0.9900
C36A—H361	0.9800	C75B—C76B	1.512 (8)
C36A—H362	0.9800	C75B—H753	0.9900

C36A—H363	0.9800	C75B—H754	0.9900
C34B—C35B	1.524 (9)	C76B—H764	0.9800
C34B—H343	0.9900	C76B—H765	0.9800
C34B—H344	0.9900	C76B—H766	0.9800
C35B—C36B	1.500 (9)	C80—C85	1.361 (6)
C35B—H353	0.9900	C80—C81	1.376 (6)
C35B—H354	0.9900	C80—H80	0.9500
C36B—H364	0.9800	C81—C82	1.358 (7)
C36B—H365	0.9800	C81—H81	0.9500
C36B—H366	0.9800	C82—C83	1.385 (6)
Sn2—O41	2.090 (2)	C82—H82	0.9500
Sn2—O42	2.628 (2)	C83—C84	1.359 (6)
Sn2—O44	2.093 (2)	C83—H83	0.9500
Sn2—O45	2.628 (2)	C84—C85	1.357 (6)
Sn2—C69	2.121 (3)	C84—H84	0.9500
Sn2—C73	2.117 (3)	C85—H85	0.9500

O1—Sn1—O4	83.18 (9)	O44—Sn2—C73	103.87 (12)
O1—Sn1—O5	137.43 (8)	O45—Sn2—C69	91.09 (11)
O1—Sn1—C29	100.36 (12)	O45—Sn2—C73	85.69 (11)
O1—Sn1—C33	106.03 (12)	C69—Sn2—C73	144.09 (13)
O2—Sn1—O4	138.10 (8)	O44—Sn2—O45	54.15 (7)
O2—Sn1—O5	167.32 (7)	O41—Sn2—O42	54.24 (8)
O2—Sn1—C29	86.01 (12)	C41—O41—Sn2	105.14 (19)
O2—Sn1—C33	89.64 (12)	C41—O42—Sn2	81.07 (19)
O4—Sn1—C29	101.81 (12)	C43—O43—H43	109.5
O4—Sn1—C33	104.98 (11)	C54—O44—Sn2	105.22 (19)
O5—Sn1—C29	88.16 (12)	C54—O45—Sn2	81.09 (19)
O5—Sn1—C33	88.50 (12)	C56—O46—H46	109.5
C29—Sn1—C33	144.16 (14)	N42—N41—C46	115.0 (3)
O1—Sn1—O2	54.94 (8)	N41—N42—C48	113.5 (3)
O4—Sn1—O5	54.28 (8)	N44—N43—C59	114.6 (3)
C1—O1—Sn1	103.6 (2)	N43—N44—C61	114.3 (3)
C1—O2—Sn1	82.0 (2)	O42—C41—O41	119.5 (3)
C3—O3—H3	109.5	O42—C41—C42	122.6 (3)
C14—O4—Sn1	105.0 (2)	O41—C41—C42	117.9 (3)
C14—O5—Sn1	81.0 (2)	C47—C42—C43	119.4 (3)
C16—O6—H6	109.5	C47—C42—C41	119.9 (3)
N2—N1—C6	114.5 (3)	C43—C42—C41	120.8 (3)
N1—N2—C8	114.8 (3)	O43—C43—C42	122.9 (3)
N4—N3—C19	113.7 (3)	O43—C43—C44	118.1 (3)
N3—N4—C21	112.9 (3)	C42—C43—C44	119.0 (3)
O2—C1—O1	119.4 (3)	C45—C44—C43	120.3 (3)
O2—C1—C2	121.7 (3)	C45—C44—H44	119.9
O1—C1—C2	118.8 (3)	C43—C44—H44	119.9
C7—C2—C3	119.0 (3)	C44—C45—C46	121.1 (3)
C7—C2—C1	120.4 (3)	C44—C45—H45	119.5
C3—C2—C1	120.6 (3)	C46—C45—H45	119.5

O3—C3—C4	117.8 (3)	C47—C46—C45	119.4 (3)
O3—C3—C2	123.1 (3)	C47—C46—N41	114.4 (3)
C4—C3—C2	119.1 (3)	C45—C46—N41	126.2 (3)
C5—C4—C3	121.0 (3)	C46—C47—C42	120.8 (3)
C5—C4—H4	119.5	C46—C47—H47	119.6
C3—C4—H4	119.5	C42—C47—H47	119.6
C4—C5—C6	120.1 (3)	C49—C48—C53	119.6 (3)
C4—C5—H5	119.9	C49—C48—N42	124.9 (3)
C6—C5—H5	119.9	C53—C48—N42	115.5 (3)
C7—C6—C5	119.5 (3)	C50—C49—C48	119.6 (3)
C7—C6—N1	116.5 (3)	C50—C49—H49	120.2
C5—C6—N1	124.0 (3)	C48—C49—H49	120.2
C6—C7—C2	121.2 (3)	C49—C50—C51	121.8 (4)
C6—C7—H7	119.4	C49—C50—H50	119.1
C2—C7—H7	119.4	C51—C50—H50	119.1
C13—C8—C9	119.6 (3)	C52—C51—C50	117.9 (3)
C13—C8—N2	115.5 (3)	C52—C51—C67	121.4 (3)
C9—C8—N2	124.9 (3)	C50—C51—C67	120.7 (4)
C10—C9—C8	119.7 (4)	C51—C52—C53	121.6 (3)
C10—C9—H9	120.1	C51—C52—H52	119.2
C8—C9—H9	120.1	C53—C52—H52	119.2
C9—C10—C11	121.3 (4)	C52—C53—C48	119.5 (4)
C9—C10—H10	119.3	C52—C53—H53	120.2
C11—C10—H10	119.3	C48—C53—H53	120.2
C10—C11—C12	118.8 (3)	O45—C54—O44	119.5 (3)
C10—C11—C27	121.3 (4)	O45—C54—C55	122.2 (3)
C12—C11—C27	120.0 (4)	O44—C54—C55	118.3 (3)
C11—C12—C13	120.2 (4)	C60—C55—C56	118.6 (3)
C11—C12—H12	119.9	C60—C55—C54	120.5 (3)
C13—C12—H12	119.9	C56—C55—C54	121.0 (3)
C8—C13—C12	120.3 (4)	O46—C56—C57	118.1 (3)
C8—C13—H13	119.8	O46—C56—C55	122.5 (3)
C12—C13—H13	119.8	C57—C56—C55	119.5 (3)
O5—C14—O4	119.4 (3)	C58—C57—C56	121.3 (3)
O5—C14—C15	122.7 (3)	C58—C57—H57	119.3
O4—C14—C15	117.9 (3)	C56—C57—H57	119.3
C20—C15—C16	118.9 (3)	C57—C58—C59	119.3 (3)
C20—C15—C14	120.0 (3)	C57—C58—H58	120.3
C16—C15—C14	121.0 (3)	C59—C58—H58	120.3
O6—C16—C17	118.0 (3)	C60—C59—C58	120.2 (3)
O6—C16—C15	122.3 (3)	C60—C59—N43	115.0 (3)
C17—C16—C15	119.8 (3)	C58—C59—N43	124.8 (3)
C18—C17—C16	120.5 (4)	C59—C60—C55	121.1 (3)
C18—C17—H17	119.7	C59—C60—H60	119.5
C16—C17—H17	119.7	C55—C60—H60	119.5
C17—C18—C19	120.0 (3)	C66—C61—C62	120.1 (3)
C17—C18—H18	120.0	C66—C61—N44	116.2 (3)
C19—C18—H18	120.0	C62—C61—N44	123.8 (3)

C20—C19—C18	119.4 (3)	C63—C62—C61	118.7 (4)
C20—C19—N3	114.6 (3)	C63—C62—H62	120.6
C18—C19—N3	126.0 (3)	C61—C62—H62	120.6
C19—C20—C15	121.3 (3)	C64—C63—C62	122.4 (4)
C19—C20—H20	119.4	C64—C63—H63	118.8
C15—C20—H20	119.4	C62—C63—H63	118.8
C26—C21—C22	119.8 (3)	C63—C64—C65	117.6 (3)
C26—C21—N4	116.1 (3)	C63—C64—C68	121.0 (4)
C22—C21—N4	124.1 (3)	C65—C64—C68	121.4 (4)
C21—C22—C23	119.5 (4)	C66—C65—C64	121.3 (4)
C21—C22—H22	120.3	C66—C65—H65	119.4
C23—C22—H22	120.3	C64—C65—H65	119.4
C24—C23—C22	120.7 (4)	C61—C66—C65	119.9 (4)
C24—C23—H23	119.7	C61—C66—H66	120.0
C22—C23—H23	119.7	C65—C66—H66	120.0
C25—C24—C23	118.7 (3)	C51—C67—H671	109.5
C25—C24—C28	120.7 (3)	C51—C67—H672	109.5
C23—C24—C28	120.6 (4)	H671—C67—H672	109.5
C26—C25—C24	120.9 (4)	C51—C67—H673	109.5
C26—C25—H25	119.5	H671—C67—H673	109.5
C24—C25—H25	119.5	H672—C67—H673	109.5
C25—C26—C21	120.4 (4)	C64—C68—H681	109.5
C25—C26—H26	119.8	C64—C68—H682	109.5
C21—C26—H26	119.8	H681—C68—H682	109.5
C11—C27—H271	109.5	C64—C68—H683	109.5
C11—C27—H272	109.5	H681—C68—H683	109.5
H271—C27—H272	109.5	H682—C68—H683	109.5
C11—C27—H273	109.5	C70—C69—Sn2	115.6 (2)
H271—C27—H273	109.5	C70—C69—H691	108.4
H272—C27—H273	109.5	Sn2—C69—H691	108.4
C24—C28—H281	109.5	C70—C69—H692	108.4
C24—C28—H282	109.5	Sn2—C69—H692	108.4
H281—C28—H282	109.5	H691—C69—H692	107.4
C24—C28—H283	109.5	C71—C70—C69	112.5 (3)
H281—C28—H283	109.5	C71—C70—H701	109.1
H282—C28—H283	109.5	C69—C70—H701	109.1
C30—C29—Sn1	117.0 (3)	C71—C70—H702	109.1
C30—C29—H291	108.1	C69—C70—H702	109.1
Sn1—C29—H291	108.1	H701—C70—H702	107.8
C30—C29—H292	108.1	C72—C71—C70	112.6 (3)
Sn1—C29—H292	108.1	C72—C71—H711	109.1
H291—C29—H292	107.3	C70—C71—H711	109.1
C29—C30—C31	110.6 (4)	C72—C71—H712	109.1
C29—C30—H301	109.5	C70—C71—H712	109.1
C31—C30—H301	109.5	H711—C71—H712	107.8
C29—C30—H302	109.5	C71—C72—H721	109.5
C31—C30—H302	109.5	C71—C72—H722	109.5
H301—C30—H302	108.1	H721—C72—H722	109.5

C32—C31—C30	112.2 (4)	C71—C72—H723	109.5
C32—C31—H311	109.2	H721—C72—H723	109.5
C30—C31—H311	109.2	H722—C72—H723	109.5
C32—C31—H312	109.2	C74B—C73—Sn2	114.5 (3)
C30—C31—H312	109.2	C74A—C73—Sn2	115.6 (4)
H311—C31—H312	107.9	C74A—C73—H731	108.4
C31—C32—H321	109.5	Sn2—C73—H731	108.4
C31—C32—H322	109.5	C74A—C73—H732	108.4
H321—C32—H322	109.5	Sn2—C73—H732	108.4
C31—C32—H323	109.5	H731—C73—H732	107.4
H321—C32—H323	109.5	C74B—C73—H733	108.6
H322—C32—H323	109.5	Sn2—C73—H733	108.6
C34A—C33—Sn1	117.5 (3)	C74B—C73—H734	108.6
C34B—C33—Sn1	117.8 (5)	Sn2—C73—H734	108.6
C34A—C33—H331	107.9	H733—C73—H734	107.6
Sn1—C33—H331	107.9	C75A—C74A—C73	118.4 (9)
C34A—C33—H332	107.9	C75A—C74A—H741	107.7
Sn1—C33—H332	107.9	C73—C74A—H741	107.7
H331—C33—H332	107.2	C75A—C74A—H742	107.7
C34B—C33—H333	107.9	C73—C74A—H742	107.7
Sn1—C33—H333	107.9	H741—C74A—H742	107.1
C34B—C33—H334	107.9	C76A—C75A—C74A	111.8 (7)
Sn1—C33—H334	107.9	C76A—C75A—H751	109.3
H333—C33—H334	107.2	C74A—C75A—H751	109.3
C33—C34A—C35A	114.9 (4)	C76A—C75A—H752	109.3
C33—C34A—H341	108.5	C74A—C75A—H752	109.3
C35A—C34A—H341	108.5	H751—C75A—H752	107.9
C33—C34A—H342	108.5	C75A—C76A—H761	109.5
C35A—C34A—H342	108.5	C75A—C76A—H762	109.5
H341—C34A—H342	107.5	H761—C76A—H762	109.5
C36A—C35A—C34A	112.4 (5)	C75A—C76A—H763	109.5
C36A—C35A—H351	109.1	H761—C76A—H763	109.5
C34A—C35A—H351	109.1	H762—C76A—H763	109.5
C36A—C35A—H352	109.1	C73—C74B—C75B	108.2 (5)
C34A—C35A—H352	109.1	C73—C74B—H743	110.1
H351—C35A—H352	107.8	C75B—C74B—H743	110.1
C35A—C36A—H361	109.5	C73—C74B—H744	110.1
C35A—C36A—H362	109.5	C75B—C74B—H744	110.1
H361—C36A—H362	109.5	H743—C74B—H744	108.4
C35A—C36A—H363	109.5	C76B—C75B—C74B	110.5 (6)
H361—C36A—H363	109.5	C76B—C75B—H753	109.5
H362—C36A—H363	109.5	C74B—C75B—H753	109.5
C33—C34B—C35B	116.3 (14)	C76B—C75B—H754	109.5
C33—C34B—H343	108.2	C74B—C75B—H754	109.5
C35B—C34B—H343	108.2	H753—C75B—H754	108.1
C33—C34B—H344	108.2	C75B—C76B—H764	109.5
C35B—C34B—H344	108.2	C75B—C76B—H765	109.5
H343—C34B—H344	107.4	H764—C76B—H765	109.5

C36B—C35B—C34B	111.0 (8)	C75B—C76B—H766	109.5
C36B—C35B—H353	109.4	H764—C76B—H766	109.5
C34B—C35B—H353	109.4	H765—C76B—H766	109.5
C36B—C35B—H354	109.4	C85—C80—C81	120.0 (5)
C34B—C35B—H354	109.4	C85—C80—H80	120.0
H353—C35B—H354	108.0	C81—C80—H80	120.0
C35B—C36B—H364	109.5	C82—C81—C80	120.9 (5)
C35B—C36B—H365	109.5	C82—C81—H81	119.5
H364—C36B—H365	109.5	C80—C81—H81	119.5
C35B—C36B—H366	109.5	C81—C82—C83	118.4 (5)
H364—C36B—H366	109.5	C81—C82—H82	120.8
H365—C36B—H366	109.5	C83—C82—H82	120.8
O41—Sn2—O44	82.81 (9)	C84—C83—C82	120.4 (5)
O41—Sn2—O45	136.85 (8)	C84—C83—H83	119.8
O41—Sn2—C69	102.61 (11)	C82—C83—H83	119.8
O41—Sn2—C73	104.03 (11)	C85—C84—C83	120.7 (5)
O42—Sn2—O44	137.00 (8)	C85—C84—H84	119.6
O42—Sn2—O45	168.83 (7)	C83—C84—H84	119.6
O42—Sn2—C69	86.48 (11)	C84—C85—C80	119.6 (5)
O42—Sn2—C73	89.90 (11)	C84—C85—H85	120.2
O44—Sn2—C69	102.97 (12)	C80—C85—H85	120.2

C6—N1—N2—C8	−178.5 (3)	Sn2—O42—C41—C42	−179.5 (3)
C19—N3—N4—C21	179.4 (3)	Sn2—O41—C41—O42	0.1 (3)
Sn1—O2—C1—O1	−2.7 (3)	Sn2—O41—C41—C42	179.5 (2)
Sn1—O2—C1—C2	176.7 (3)	O42—C41—C42—C47	−179.0 (3)
Sn1—O1—C1—O2	3.4 (3)	O41—C41—C42—C47	1.6 (4)
Sn1—O1—C1—C2	−176.0 (2)	O42—C41—C42—C43	1.2 (5)
O2—C1—C2—C7	−177.5 (3)	O41—C41—C42—C43	−178.2 (3)
O1—C1—C2—C7	1.8 (4)	C47—C42—C43—O43	−179.8 (3)
O2—C1—C2—C3	2.1 (5)	C41—C42—C43—O43	0.1 (5)
O1—C1—C2—C3	−178.5 (3)	C47—C42—C43—C44	−0.5 (5)
C7—C2—C3—O3	179.8 (3)	C41—C42—C43—C44	179.4 (3)
C1—C2—C3—O3	0.2 (5)	O43—C43—C44—C45	−179.6 (3)
C7—C2—C3—C4	−0.2 (5)	C42—C43—C44—C45	1.0 (5)
C1—C2—C3—C4	−179.8 (3)	C43—C44—C45—C46	−0.6 (5)
O3—C3—C4—C5	−179.3 (3)	C44—C45—C46—C47	−0.4 (5)
C2—C3—C4—C5	0.6 (5)	C44—C45—C46—N41	−179.4 (3)
C3—C4—C5—C6	−0.9 (5)	N42—N41—C46—C47	174.7 (3)
C4—C5—C6—C7	0.7 (5)	N42—N41—C46—C45	−6.3 (4)
C4—C5—C6—N1	−179.3 (3)	C45—C46—C47—C42	1.0 (5)
N2—N1—C6—C7	−177.7 (3)	N41—C46—C47—C42	−179.9 (3)
N2—N1—C6—C5	2.3 (5)	C43—C42—C47—C46	−0.6 (5)
C5—C6—C7—C2	−0.3 (5)	C41—C42—C47—C46	179.6 (3)
N1—C6—C7—C2	179.7 (3)	N41—N42—C48—C49	−2.2 (5)
C3—C2—C7—C6	0.0 (5)	N41—N42—C48—C53	177.9 (3)
C1—C2—C7—C6	179.6 (3)	C53—C48—C49—C50	0.3 (5)
N1—N2—C8—C13	179.6 (3)	N42—C48—C49—C50	−179.5 (3)

N1—N2—C8—C9	−0.6 (5)	C48—C49—C50—C51	−0.1 (5)
C13—C8—C9—C10	−1.3 (5)	C49—C50—C51—C52	−0.6 (5)
N2—C8—C9—C10	179.0 (3)	C49—C50—C51—C67	179.6 (3)
C8—C9—C10—C11	−0.2 (5)	C50—C51—C52—C53	1.0 (5)
C9—C10—C11—C12	1.4 (5)	C67—C51—C52—C53	−179.2 (3)
C9—C10—C11—C27	−178.8 (3)	C51—C52—C53—C48	−0.8 (5)
C10—C11—C12—C13	−1.2 (5)	C49—C48—C53—C52	0.1 (5)
C27—C11—C12—C13	179.0 (3)	N42—C48—C53—C52	179.9 (3)
C9—C8—C13—C12	1.5 (5)	Sn2—O45—C54—O44	−1.3 (3)
N2—C8—C13—C12	−178.8 (3)	Sn2—O45—C54—C55	179.2 (3)
C11—C12—C13—C8	−0.2 (5)	Sn2—O44—C54—O45	1.6 (3)
Sn1—O5—C14—O4	4.2 (3)	Sn2—O44—C54—C55	−178.8 (2)
Sn1—O5—C14—C15	−174.9 (3)	O45—C54—C55—C60	178.9 (3)
Sn1—O4—C14—O5	−5.4 (3)	O44—C54—C55—C60	−0.6 (4)
Sn1—O4—C14—C15	173.7 (2)	O45—C54—C55—C56	−0.7 (5)
O5—C14—C15—C20	178.7 (3)	O44—C54—C55—C56	179.8 (3)
O4—C14—C15—C20	−0.3 (4)	C60—C55—C56—O46	−179.9 (3)
O5—C14—C15—C16	2.9 (5)	C54—C55—C56—O46	−0.3 (5)
O4—C14—C15—C16	−176.1 (3)	C60—C55—C56—C57	−0.4 (4)
C20—C15—C16—O6	179.8 (3)	C54—C55—C56—C57	179.2 (3)
C14—C15—C16—O6	−4.3 (5)	O46—C56—C57—C58	179.1 (3)
C20—C15—C16—C17	−0.8 (5)	C55—C56—C57—C58	−0.4 (5)
C14—C15—C16—C17	175.1 (3)	C56—C57—C58—C59	0.9 (5)
O6—C16—C17—C18	−178.7 (3)	C57—C58—C59—C60	−0.5 (5)
C15—C16—C17—C18	1.9 (5)	C57—C58—C59—N43	178.4 (3)
C16—C17—C18—C19	−1.2 (5)	N44—N43—C59—C60	−173.1 (3)
C17—C18—C19—C20	−0.6 (5)	N44—N43—C59—C58	8.0 (5)
C17—C18—C19—N3	−179.1 (3)	C58—C59—C60—C55	−0.2 (5)
N4—N3—C19—C20	−179.5 (3)	N43—C59—C60—C55	−179.3 (3)
N4—N3—C19—C18	−0.9 (5)	C56—C55—C60—C59	0.7 (5)
C18—C19—C20—C15	1.7 (5)	C54—C55—C60—C59	−178.9 (3)
N3—C19—C20—C15	−179.6 (3)	N43—N44—C61—C66	−175.9 (3)
C16—C15—C20—C19	−1.0 (5)	N43—N44—C61—C62	4.4 (5)
C14—C15—C20—C19	−176.9 (3)	C66—C61—C62—C63	−1.5 (5)
N3—N4—C21—C26	173.7 (3)	N44—C61—C62—C63	178.2 (3)
N3—N4—C21—C22	−8.1 (5)	C61—C62—C63—C64	1.2 (5)
C26—C21—C22—C23	−0.5 (5)	C62—C63—C64—C65	−0.5 (5)
N4—C21—C22—C23	−178.7 (3)	C62—C63—C64—C68	−179.6 (3)
C21—C22—C23—C24	−0.5 (5)	C63—C64—C65—C66	0.2 (5)
C22—C23—C24—C25	0.7 (5)	C68—C64—C65—C66	179.3 (3)
C22—C23—C24—C28	−179.3 (3)	C62—C61—C66—C65	1.2 (5)
C23—C24—C25—C26	0.1 (5)	N44—C61—C66—C65	−178.5 (3)
C28—C24—C25—C26	−179.9 (3)	C64—C65—C66—C61	−0.5 (5)
C24—C25—C26—C21	−1.1 (5)	Sn2—C69—C70—C71	−72.9 (4)
C22—C21—C26—C25	1.3 (5)	C69—C70—C71—C72	178.3 (3)
N4—C21—C26—C25	179.6 (3)	Sn2—C73—C74A—C75A	55.7 (8)
Sn1—C29—C30—C31	−75.0 (4)	C73—C74A—C75A—C76A	65.6 (16)
C29—C30—C31—C32	177.9 (4)	Sn2—C73—C74B—C75B	−77.7 (9)

Sn1—C33—C34A—C35A	−69.3 (7)	C73—C74B—C75B—C76B	−176.5 (9)
C33—C34A—C35A—C36A	−178.3 (7)	C85—C80—C81—C82	−0.3 (7)
Sn1—C33—C34B—C35B	49.1 (11)	C80—C81—C82—C83	−0.2 (7)
C33—C34B—C35B—C36B	80 (2)	C81—C82—C83—C84	1.3 (7)
C46—N41—N42—C48	179.5 (3)	C82—C83—C84—C85	−2.0 (7)
C59—N43—N44—C61	−177.5 (3)	C83—C84—C85—C80	1.5 (7)
Sn2—O42—C41—O41	−0.1 (3)	C81—C80—C85—C84	−0.4 (7)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O2	0.84	1.88	2.618 (3)	145
O6—H6···O5	0.84	1.89	2.631 (3)	146
O43—H43···O42	0.84	1.90	2.635 (3)	146
O46—H46···O45	0.84	1.91	2.627 (3)	142
C28—H281···O4^{i}	0.98	2.56	3.385 (5)	142
C73—H733···O41^{ii}	0.99	2.58	3.540 (5)	162
C30—H301···*Cg*7	0.99	2.83	3.717 (5)	149
C34*A*—H341···*Cg*4^{iii}	0.99	2.64	3.586 (5)	160
C34*B*—H344···*Cg*4^{iii}	0.99	2.73	3.662 (13)	157
C70—H702···*Cg*6^{iii}	0.99	2.71	3.654 (4)	159
C74*A*—H741···*Cg*9^{ii}	0.99	2.69	3.643 (7)	161
C74*B*—H743···*Cg*9^{ii}	0.99	2.83	3.692 (7)	146

Symmetry codes: (i) −*x*+1, −*y*, −*z*; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*, *y*+1, *z*.